

# CHEMICAL ENGINEERING

December  
2019

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Waste Treatment

Production of Ethylene Oxide

# Tips for Tanks and Vessels

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Chemical  
Engineering  
Buyer's Guide  
**2020**

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## Coming in January

Look for: **Feature Reports** on Sampling for Process Analytics; and Evaporators; A **Focus** on Motors & Drives; A **Facts at your Fingertips** on Air-Pollution Control; **News Articles** on the Kirkpatrick Chemical Engineering Achievement Award; and Particle-Size Control; **New Products**; and much more

**Cover design:** Rob Hudgins



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## Pursuing the potential of hydrogen

Hydrogen's potential for playing a significant role in the global search for clean, secure energy sources is garnering much attention from a growing number of industries and governments. Driven by concerns about climate change, investors as well as policy makers are pushing for aggressive carbon reductions.

As a fuel, hydrogen offers the advantage of producing no greenhouse gases upon combustion. The bulk of the world's hydrogen supply, however, is produced from fossil fuels and is currently being used industrially mostly for the petroleum refining and fertilizer industries. According to the International Energy Agency<sup>1</sup> (IEA; www.iea.org), the production of hydrogen generates about 830 million metric tons per year of CO<sub>2</sub> emissions. There is, however, a surge in projects to create "green" hydrogen from water via electrolysis.

### 'Green' hydrogen

Renewable energy sources, such as wind and solar energy, or nuclear power, can be used to generate hydrogen by electrolysis, making it an attractive option for storing the variable output from these sources. According to Dave Wolff, eastern region manager at Nel Hydrogen<sup>2</sup> (www.nelhydrogen.com), electrolysis equipment prices are dropping, and that combined with decreasing costs of renewable energy makes the green route to hydrogen more economically attractive than it has been in the past.

Last month, voestalpine AG (www.voestalpine.com) and partners commenced operation of what is currently the world's largest pilot plant for green hydrogen production in Linz, Austria, with a capacity of over 6 MW. The project receives €18 million in E.U. funding and will test whether the technology is suitable for industrial scale, as well as the potential to compensate for fluctuations in the power grid.

In another project, Salzgitter Flachstahl GmbH (www.salzgitter-ag.com) is planning to build a 2.2-MW electrolysis plant, which is expected to cover the company's entire hydrogen demand for steel-making. Seven wind turbines will generate the needed electric power. The plant is due to start operations in the 4th quarter of 2020.

### Mobility and more

Hydrogen also has the potential to play a significant role in power generation and transportation. Air Liquide (www.airliquide.com), Engie and the Durance, Luberon, Verdon urban area (DLVA) entered into a partnership last month on a project that will develop the technological and economic conditions for producing 1,300 GWh of solar electricity together with the production of green hydrogen. The ambitious plan anticipates eventual large quantities of green hydrogen that could be produced for uses including energy, industry and mobility applications.

Last year, Anheuser-Busch placed an order with Nikola Motor Co. for up to 800 hydrogen-electric powered semi-trucks. The company expects to start integrating the vehicles into its fleet beginning in 2020, and to convert its full long-haul fleet to renewable-powered trucks by 2025.

While hydrogen has received attention as a clean energy source in the past, the current momentum fueled by decarbonization goals and improved technologies shows greater promise for realizing its potential. ■

*Dorothy Lozowski, Editorial Director*



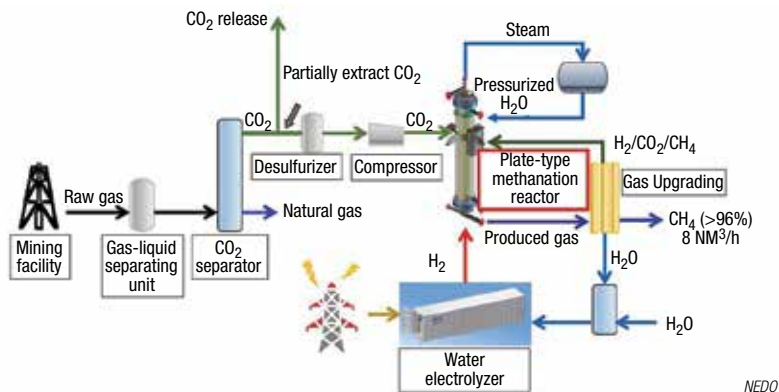
1. IEA, The Future of Hydrogen: Seizing today's opportunities, June 2019, www.iea.org.
2. Nel Hydrogen, Webinar presented on November 19, 2019 by Dave Wolff, www.chemengonline.com/webinars.

## Pursuing methanation as a means to recycle CO<sub>2</sub>

By the end of fiscal 2019, commissioning and continuous operation will begin on a new methanation plant that will produce 8 Nm<sup>3</sup>/h of methane from CO<sub>2</sub> and H<sub>2</sub>. The test facility, located at the Koshijihara Plant of

Inpex's Nagaoka Field Office in Nagaoka City, Niigata Prefecture, is part of an industry-government collaboration led by the New Energy and Industrial Technology Development Organization (NEDO; Kawasaki City, Japan; [www.nedo.go.jp](http://www.nedo.go.jp)), with partners Inpex Corp. (Tokyo; [www.inpex.co.jp](http://www.inpex.co.jp)) and Hitachi Zosen Corp. (both Tokyo; [www.hitachizosen.co.jp](http://www.hitachizosen.co.jp)).

In the project (diagram), the partners aim to use this test facility to further develop methanation technology, which is one method for recycling CO<sub>2</sub>. For feedstock, the plant will use CO<sub>2</sub> recovered from natural-gas processing at the Koshijihara Plant, and H<sub>2</sub> generated from water electrolysis using renewable electricity. The product



methane is said to have a great potential as an energy carrier, and offers significant benefits because existing infrastructure for natural gas can be employed directly.

Through later full-scale operation, the partners aim to evaluate and examine technical issues, including how to optimize the methane synthesis process by varying a range of parameters, including reaction temperature, reaction pressure and reaction loads, and to develop methanation technology. For methane synthesis, the test facility uses a Hitachi Zosen plate reactor that achieves highly efficient heat recovery. As the world's first trial using actual CO<sub>2</sub> in a plate reactor, this initiative is focused on the use of larger facilities in the future.

## Lower-cost engineered composites for transportation infrastructure applications

Engineered cementitious composites (ECCs) are concrete-like materials with exceptional ductility (up to 500 times) and flexural strengths (2–3 times) greater than conventional concrete. The flexibility and strength of ECCs could benefit transportation infrastructure (for example, the ductility of ECCs could reduce or eliminate the need to cut joints into roadway repair overlays, which reduces repair times and cost).

However, current ECCs require difficult-to-obtain materials (such as microsilica sand) and are expensive to manufacture (due to high fiber content). "The only way to make ECCs applicable in the real world is to figure out how to make them from cost-effective and readily available materials," explains Gabriel Arce, engineering research assistant professor at Louisiana State University (Baton Rouge, La.; [www.lsu.edu](http://www.lsu.edu)). Arce leads a group of researchers that is evaluating different ingredients in ECC formulations to modify its properties, increase its cost-

effectiveness or reduce its carbon footprint.

The LSU team recently substituted sugarcane bagasse ash (SCBA) for the microsilica sand and found that strength and ductility of the ECC could be retained or even enhanced. "The degree of enhancement depends on the amount of sand replacement with SCBA and the type of processing to which the SCBA is subjected," Arce says. "We have managed to replace up to 100% of sand with SCBA with promising results."

The group also demonstrated the ability to manufacture one of its lower-cost ECC formulations (utilizing locally available fine river sand and low fiber content), in amounts sufficient to make two 60-ft long overlay sections to repair a deteriorated asphalt pavement at the Louisiana Dept. of Transportation and Development (DOTD) Pavement Research Facility.

The LSU group is also investigating the partial substitution of Portland cement with SCBA, and has begun a collaborative project to develop geopolymer-based ECCs with Texas A&M University.

Edited by:  
**Gerald Ondrey**

### DIRECT ROUTE TO PG

Dow Inc. (Midland, Mich.; [www.dow.com](http://www.dow.com)) and Evonik Industries AG (Essen, Germany; [www.evonik.com](http://www.evonik.com)) have entered into an exclusive technology partnership to develop a new process to make propylene glycol (PG). The key to the so-called Hyprosyn process is a catalytic system developed by Evonik researchers that allows for the direct synthesis of PG from propylene and hydrogen peroxide, in a process offering high yield and comparatively low energy consumption. A pilot plant is to be constructed at the Evonik site in Hanau, Germany by the end of 2020, with large-scale technical implementation to follow a few years later.

In the traditional process, propylene oxide (PO) is converted to PG using water. According to Evonik, the Hyprosyn technology offers several advantages over that process: it is expected to consume significantly less energy while providing a higher yield; the Hyprosyn process combines all reaction steps in a single reactor, eliminating the need for investment in additional PO capacity; and only H<sub>2</sub>O<sub>2</sub> and propylene are processed as feedstock.

### ETHYLENE AMINES

Nouryon (Amsterdam, the Netherlands; [www.nouryon.com](http://www.nouryon.com)) has inaugurated a demonstration plant in Stenungsund, Sweden to demonstrate a new, more sustainable technology platform to produce ethylene amines and their derivatives. The technology, which is based on ethylene oxide (EO), allows for selective production of a wide range of end products. The company has successfully produced the first ethylene amines products in the demonstration plant, confirming the new technology.

(Continues on p. 6)

ogy on an industrially relevant scale and marking the next step toward full commercialization. Front-end engineering design (FEED) activities for a world-scale manufacturing facility based on this new technology are expected to start by the end of 2019.

## COLD ENERGY STORAGE

Highview Power (London, U.K.; [www.highviewpower.com](http://www.highviewpower.com)) plans to construct the U.K.'s first large-scale commercial cryogenic-energy storage facility, which will be located at a decommissioned thermal-power station in the North of England. The 50 MW/250 MWh project will be the first large-scale energy storage facility to use the company's CryoBattery technology, which was first demonstrated in a 5-MW plant in Pilsforth, Greater Manchester, and has been successfully operating since early 2018.

The CryoBattery consists of three steps. For charging, air is cleaned and dried and then refrigerated (using off-peak or excess electricity) by a series of compression and expansion stages (Claude cycle) to produce liquefied air at  $-196^{\circ}\text{C}$ . The liquid air is stored in insulated tanks at low pressure. When power is required, the liquid air is pumped to high pressure and heated, and the expanded gas drives a turbine to generate electricity.

According to the company, the CryoBattery is the only freely locatable energy-storage solution on the market today that delivers clean, reliable and cost-efficient, long-duration energy storage with grid synchronous inertia. It can store energy for weeks, instead of hours or days, and at approximately £110/MWh for a for a 10-h, 200-MW/2-GWh system, the CryoBattery offers the lowest levelized cost of storage for large-scale applications.

## CALCIUM BATTERIES

Efficient, large and low-cost energy storage systems will facilitate Germany's transition to zero-emission mobility and power. Today's predominant

## Geothermal brine may be a new U.S. source of lithium . . .

**C**urrently the U.S. has only one domestic source of lithium, a vital element in lithium-ion batteries and other products, but this could be changed through processes being developed by two California companies. Furthest along is a project of EnergySource Minerals LLC (San Diego, Calif.; [www.energysource.us.com](http://www.energysource.us.com)) to obtain lithium from geothermal brine. The company has a pilot plant at a geothermal power plant near Southern California's Salton Sea, where its affiliate, EnergySource, produces electricity by pumping geothermal brine of about  $500^{\circ}\text{F}$  and 500 psig through wells and flashing it to produce steam for turbines.

The brine contains about 25–30% solids, including about 250 parts per million (ppm) of lithium. Silica is managed by a crystallizer-

clarifier process and the spent brine, containing dissolved solids, is reinjected into the ground. In the lithium process, clarified brine is purified, then lithium is selectively extracted by a proprietary adsorbent and recovered by a water wash. The process is continuous and the plant design is mechanically simple, with multiple columns controlled by a single valve, says Derek Benson, EnergySource's chief operating officer. "We get high lithium recovery and very high rejection of unwanted dissolved solids."

Lithium is recovered as lithium chloride, but Benson says the final product will probably be lithium hydroxide, which is replacing lithium carbonate as the favored material for batteries. EnergySource Minerals plans to activate a commercial plant producing about 19,000 m.t./yr in early 2023.

## . . . and this process may produce lithium from borate process waste

**M**eanwhile, Rio Tinto (London, U.K.; [www.riotinto.com](http://www.riotinto.com)) will shortly start up a pilot plant to produce battery-grade lithium carbonate from 90 years' accumulated plant waste at its U.S. Borax operation in Boron, Calif. The waste is clay from the production of borates, in which borax ore is crushed and mixed with hot water to dissolve the borates, then the undissolved solids are screened out.

The waste contains about 2,000 ppm of

lithium, says Richard Cohen, managing director of borates and lithium. Rio Tinto recovers the lithium by roasting and leaching. Cohen declines to give further details, but a conventional method is to use dilute sulfuric acid to leach lithium from ore. Rio Tinto says the process has been proved on a small scale and will be optimized in a pilot plant that will produce 10-m.t./yr of lithium-carbonate equivalent. The process is expected to have an economic advantage, since the metal has already been mined.

## A microbe for making chemicals from brown algae

**A** research team from Pohang University of Science and Technology (Pohang, South Korea; [www.postech.ac.kr](http://www.postech.ac.kr)), led by professor Gyoo Yeol Jung, and Seoul National University (Seoul, South Korea; [www.useoul.edu](http://www.useoul.edu)), led by professor Sang Woo Seo, has developed a new microorganism — dubbed *Vibrio sp. dhg* — that can be a promising platform for producing biofuels with brown macroalgae.

Extensive studies have been conducted to utilize non-edible biomass as a feedstock for producing fuels and other useful bioproducts and brown macroalgae has been seen as an alternative feedstock. Brown macroalgae grow up to three times faster than the starch crops and only require light and seawater to grow.

The most prominent sugars in brown macroalgae are alginate and mannitol. The utilization of brown macroalgae by conventional microbial platforms has been limited due to the

inability to metabolize one of the principal sugars, alginate (a copolymer of  $\alpha$ -L-gulonate and  $\beta$ -D-mannuronate). While conventional microbial platforms such as *Escherichia coli* can easily metabolize mannitol, its ability to assimilate alginate is hindered by the fact that it lacks certain related genes. Although *E. coli* can be engineered to utilize alginate, its growth rate and metabolic activity are still too low for industrial application.

The team established a genetic toolbox for the engineering of *Vibrio sp. dhg*. It also demonstrated the new microorganism's ability to rapidly produce ethanol (a biofuel); 2,3-butanediol (a raw material for plastics); and lycopene (a physiologically active substance) from brown macroalgae/sugar mixture with high productivity and yield.

The new microorganism is expected to enhance the efficiency of the microbial fermentation process using not only algae, but also conventional glucose-based biomass.

(Continues on p. 8)



lithium-ion technology, however, cannot fulfill this task on a global scale, says Maximilian Fichtner, professor at the Karlsruhe Institute of Technology (KIT; Germany; [www.kit.edu](http://www.kit.edu)) and director of the research platform CELEST (Center for Electrochemical Energy Storage; Ulm & Karlsruhe). "In the medium term, Li-ion batteries will reach their limits in terms of performance and some of the resources used for their manufacture ... Availability of resources needed for manufacture, such as cobalt, nickel and lithium, is limited," he says. At the Helmholtz Institute Ulm, established by KIT in cooperation with Ulm University, Fichtner and his team focus on alternative battery technologies that are based on more abun-

(Continues on p. 10)

## Novel catalyst for transforming polyethylene into lubricants and waxes

Efficient upcycling of post-consumer plastics, such as polyethylene (PE), is a key sustainability objective. New research by a team at Argonne National Laboratory (Argonne, Ill.; [www.anl.gov](http://www.anl.gov)) and Ames Laboratory (Ames, Iowa; [www.ameslab.gov](http://www.ameslab.gov)) has resulted in a novel catalyst material that can transform linear polyethylene into a narrow range of liquid hydrocarbons that could be used for making lubricating oils and wax intermediates for surfactants. The research could eventually create a path for generating value-added products from used polyolefins, a currently untapped resource.

The Argonne/Ames team, along with collaborators from academia, built a catalyst that consists of two-nanometer platinum particles held in place by strontium titanate ( $\text{SrTiO}_3$ ) nanocuboids that are an order of magnitude larger (100 nm). The  $\text{SrTiO}_3$  is similar to perovskite, and was chosen because it can remain stable under the elevated

temperatures and pressures required for the reaction to break C–C bonds in the PE.

To place the platinum nanoparticles, the researchers used atomic layer deposition, a technique developed at Argonne and Northwestern University (Evanston, Ill.; [www.northwestern.edu](http://www.northwestern.edu)) that allows precise control over the size of the nanoscale particles.

In a recently published paper in *ACS Cent. Sci.*, the team reported the effectiveness of the catalyst for converting PE into liquid hydrocarbons in a narrow molecular-weight distribution and found that certain nanoparticle structures (higher edge-to-face ratio) performed better. The group successfully tested the catalyst on research-grade PE and on post-consumer plastic bags at laboratory scale. A critical aspect of the catalyst is its ability to selectively break C–C bonds in longer chains in preference to shorter chains, allowing the narrow range of products without forming light hydrocarbons.

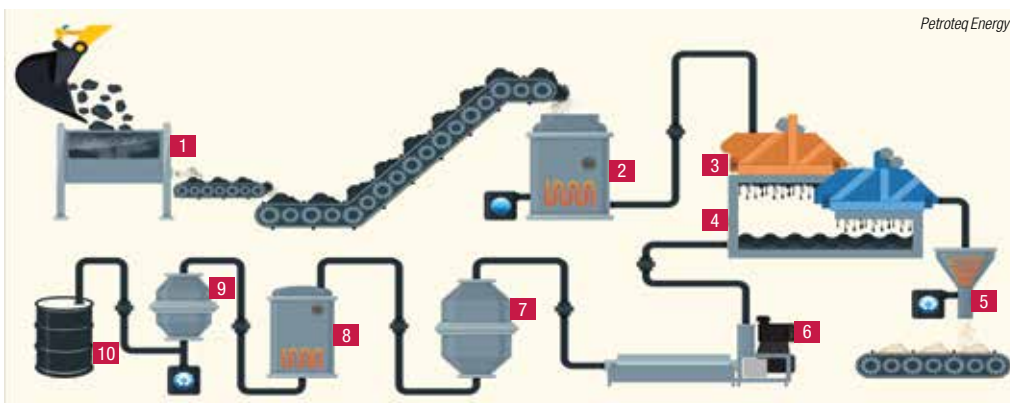
## Solvent chemistry is key for cleaner oil-sands processing

Petroteq Energy Inc. (Sherman Oaks, Calif.; [www.petroteq.energy](http://www.petroteq.energy)) has achieved continuous operation at its oil-sands processing site in Utah, which is said to be the first commercial plant in the U.S. to extract and upgrade crude oil from U.S. oil sands. Petroteq has developed a closed-loop extraction process (diagram), known as Clean Oil Recovery Technology (CORT), which employs a proprietary low-boiling-point solvent. The solvent, which is composed of hydrophobic, hydrophilic and polycyclic hydrocarbons, can dissolve up to 99% of the oil sands' hydrocarbon content, while also enabling operation at much milder temperatures and pressures than traditional methods for processing oil sands. "The solvent forms an azeotropic mixture, which allows for more economical solvent recovery. We can recycle up to 99% of the solvent," explains Vladimir Podlipskiy, Petroteq Energy chief technology officer. "Furthermore, CORT can extract very small clay particles from the oil sands, which minimizes the formation of problematic clay emulsions and prevents equipment clog-

ging," he adds.

"The ability to recycle the solvent within the process avoids water consumption and enables a lower overall footprint, since tailing ponds are eliminated — an advantage over traditional mining technologies, which typically use extremely large volumes of water," points out David Sealock, Petroteq chief executive officer.

After five years of scaleup work, Petroteq recently began operating two 500-bbl/d trains in Utah, producing a crude heavy oil product that meets the quality demands for diesel fractionation. "We also have a 3,000-bbl/d application approved by the Department of Oil, Gas and Mining in Utah. We hope to have that running in early 2021," adds Sealock. In addition to processing



### Legend:

1. Oil sands are crushed
2. Raw ore mixed with first-phase solvent
3. First-phase sand-separation process removes sand; integrated with phase-four oil and solvent extraction
4. Fluid separation extraction
5. Newly added augers produce clean sand; solvent and oil captured and recycled
6. Sediment extraction unit
7. Fluid heated to separate solvent from oil
8. Secondary extraction column
9. Evaporated solvent recycled
10. Heavy oil product

oil sands, Sealock says that CORT can be tailored for any application that requires removal of hydrocarbons from soil. "We can extract up to 99% of hydrocarbons out of soil. For reclamation and remediation, we can clean up any soil that has been contaminated with hydrocarbons, including at old refinery locations, tailing ponds or anywhere with a massive spill," he adds.

## 'Electro-swing' adsorption separates CO<sub>2</sub> from mixed gases at any concentration

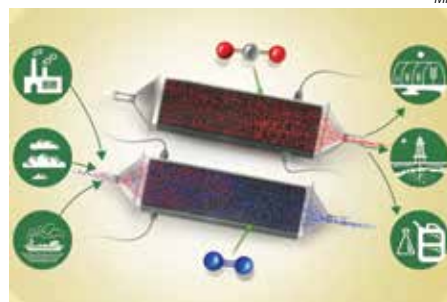
Effectively separating carbon dioxide from combustion exhaust or directly from air is essential for realizing net reductions in greenhouse-gas emissions, but existing technologies for CO<sub>2</sub> capture (such as CO<sub>2</sub>-scrubbing with amines), involve parasitic energy losses, which make carbon-capture economics unfavorable. To address this, researchers from the laboratory of T. Alan Hatton at the Massachusetts Institute of Technology (MIT; Cambridge, Mass.; [www.mit.edu](http://www.mit.edu)) Department of Chemical Engineering have demonstrated the first voltage-dependent separation of CO<sub>2</sub> from mixed-gas using electro-swing adsorption (ESA).

MIT's device is an electrochemical cell that selectively captures CO<sub>2</sub> when current is applied in one direction, and releases CO<sub>2</sub> when the current is reversed. The ESA system takes advantage of the fact that the molecule quinone, in its two reduced forms, reacts

with CO<sub>2</sub> in a nucleophilic addition, but has no affinity for CO<sub>2</sub> in its oxidized form, explains Sahag Voskian, a post-doctoral researcher at MIT. "It is this binary nature of the affinity of quinone to CO<sub>2</sub> at its different oxidation states which makes this system unique," Voskian notes.

The researchers synthesized cathode material by polymerizing quinone and suspending the polyquinone in a solution of dispersed carbon nanotubes (CNTs). The polyquinone-CNT "ink" is used to dip-coat the cathode, Voskian says, and a ferrocene-CNT anode allows for reversible charge-discharge of the cell (that is, capture and release of the CO<sub>2</sub>). Ionic liquids serve as electrolytes to complete the circuit.

A series of five-layer electrode sheets are arranged in parallel such that the CO<sub>2</sub>-containing mixed gas flows through the channels between the stationary stacks (diagram). The cell architecture is designed to maximize contact between the gas and




the high-surface-area electrodes.

The device works at ambient conditions on a wide range of CO<sub>2</sub> concentrations in the feed gas, from parts-per-million (ppm)-level CO<sub>2</sub> to 100% CO<sub>2</sub>, and can be controlled to release pure CO<sub>2</sub> for other applications or for long-term underground disposal, Voskian says.

Voskian and Hatton, along with Brian Baynes, founded a company to develop prototypes for the device, optimize the electrode manufacturing process and eventually build a pilot plant.



dant resources. Calcium is a promising candidate, because it can release and accept two electrons per atom contrary to lithium and because it supplies a voltage similar to that of lithium: “Calcium is the fifth most abundant element in the Earth’s crust. It is distributed homogeneously on Earth and it is safe, non-toxic, and inexpensive,” Fichtner says.

In contrast to the established Li-ion technology or more recent sodium or magnesium technologies, practicable electrolytes to produce rechargeable calcium batteries have been lacking so far. Now, the researchers have succeeded in synthesizing a class of new electrolytes based on organic calcium salts. These electrolytes enable charging at room temperature. Using the new electrolyte calcium tetrakis[hexafluoroisopropoxy] borate, the researchers demonstrated feasibility of calcium batteries of high energy density, storage capacity, and quick-charging capability. Their results are reported in the journal *Energy & Environmental Science*. 


## Machine learning helps achieve a five-fold boost in formaldehyde yield

**C**hemistry professor Oliver Trapp and his colleagues at the Ludwig-Maximilians-Universität München (LUM; Germany; [www.en.uni-muenchen.de](http://www.en.uni-muenchen.de)) have developed a new workflow for the production of formaldehyde, which is based on an algorithm constructed with the aid of machine learning (ML), optimization and design of experiments (DoE). The new procedure increases yields of the compound by a factor of five, as the team recently reported in the journal *Chemical Science*.

Industrial synthesis of formaldehyde begins with synthesis gas (syngas), to which methanol is added before being oxidized with the help of a catalyst. However, the production of syngas itself requires high temperatures and fossil fuels such as natural gas or coal. In a previous study, the LMU researchers described the development of a reaction scheme that allowed dimethoxymethane (DMM) — a formaldehyde derivative that can be hydrolyzed into formaldehyde and methanol — to be synthesized in a single step from syngas in the presence of a ruthenium-based catalyst,

under moderate conditions of temperature and pressure. The strategy has a number of advantages over the conventional procedure. First, it allows CO<sub>2</sub> to be utilized. “In addition, the whole process requires far less energy than alternative routes of synthesis, as it occurs at lower temperatures and involves fewer steps,” says Trapp.

The group has now optimized its procedure by varying seven parameters that affect the yield of formaldehyde synthesis in their system, and using ML to identify the parameter combinations that give the best results. By appropriately tuning the input parameters in a new reaction setup, they were able to test the efficacy of the algorithm directly. “The new reaction scheme increased the efficiency of synthesis by 500% relative to that of the conventional mode of formaldehyde production,” says Trapp.

The authors are confident that their results will motivate chemical engineers to adopt the process and implement it on a technical scale. “BASF, our partner in the project, is already engaged in assessing the industrial relevance of the process,” says Trapp. 

## Plant Watch

### Wacker starts up new silicon-metal production plant in Norway

November 15, 2019 — Wacker Chemie AG's (Munich, Germany; [www.wacker.com](http://www.wacker.com)) new silicon-metal production plant officially went on stream at the Holla site in Norway, following over two years of construction. The new furnace is one of the largest of its kind in the world and increases the Holla site's total capacity by more than 40%. A total of around €100 million was invested in the new plant.

### Teijin Aramid moves forward with capacity expansion

November 13, 2019 — Teijin Aramid B.V. (Arnhem, the Netherlands; [www.teijinaramid.com](http://www.teijinaramid.com)) began a second round of activities to increase para-aramid fiber production, targeting more than 25% capacity increase in five years. After the first phase of expansion through debottlenecking, the company now moves into the major phase of investment, realizing the full increased capacity by 2022. The expansion projects will take place in two plants in Delfzijl and Emmen, the Netherlands. Delfzijl is the production site for monomers and polymers, and the Emmen plant is used for spinning.

### McDermott wins AMS technology contract from Formosa Chemicals

November 8, 2019 — McDermott International, Inc. (Houston; [www.mcdermott.com](http://www.mcdermott.com)) has been awarded a technology contract by Formosa Chemicals Industries Ningbo Ltd. for an alpha-methylstyrene (AMS) recovery unit in Ningbo, China. This will utilize AMS technology jointly licensed by Versalis (San Donato Milanese, Italy; [www.versalis.eni.com](http://www.versalis.eni.com)) and McDermott's Lummus Technology to recover 10,000 metric tons per year (m.t./yr) of AMS.

### Avantium opens plant-based MEG demonstration plant

November 7, 2019 — Avantium (Amsterdam, the Netherlands; [www.avantium.com](http://www.avantium.com)) has inaugurated its plant-based monoethylene glycol (MEG) demonstration factory in Chemie Park in Delfzijl, the Netherlands. The demonstration plant has an industrially relevant capacity of 10 m.t./yr, and will also produce plant-based monopropylene glycol. Avantium says it is planning construction of a commercial plant aimed for startup in 2024.

### Perstorp breaks ground in India to significantly boost Penta business

November 7, 2019 — Perstorp AB (Malmö, Sweden; [www.perstorp.com](http://www.perstorp.com)) has unveiled plans to invest in the construction of a new pentaerythritol (Penta) production facility in Gujarat, India. Construction of the Gujarat plant started

in October 2019, with commercial production planned to start in early 2022. The site is designed to produce 40,000 m.t./yr of Penta, which is used in coatings, lubricants and antioxidants.

### Hexion to expand phenolic resin production capacity in Australia

November 6, 2019 — Hexion Inc. (Columbus, Ohio; [www.hexion.com](http://www.hexion.com)) plans to add phenolic resin capacity as the latest expansion of its adhesives and binders business at its Brimbank, Australia site. Construction of the new reactor and associated infrastructure is expected to begin in early 2020 and is expected to come online in the first quarter of 2021.

### Showa Denko to begin commercial production of 1,3-butylene glycol

November 5, 2019 — Showa Denko K.K. (SDK; Tokyo; [www.sdk.co.jp](http://www.sdk.co.jp)) has decided to commercialize 1,3-butylene glycol (1,3-BG), which is mainly used as raw material for cosmetics. SDK will finish installation of facilities to produce 1,3-BG in its Oita Complex in Japan by the end of 2019, and plans to start sale of the product in April 2020.

### Linde starts up two air-separation units at Taixing Jinyan ethylene oxide facility

October 29, 2019 — Linde plc (Guildford, U.K.; [www.linde.com](http://www.linde.com)) started up two plants to supply oxygen and nitrogen to Taixing Jinyan Chemical Technology Co. to support the production of ethylene oxide. The plants, with total combined production capacity of 29,000 Nm<sup>3</sup>/h, will also supply gases to other customers in the Taixing Economic Development Zone.

### Umicore opens new facility in Korea for the production of fuel-cell catalysts

October 23, 2019 — Umicore N.V. (Brussels, Belgium; [www.umicore.com](http://www.umicore.com)) inaugurated its new production facility for fuel-cell catalysts in SongDo Incheon City (near Seoul), South Korea. The facility will support the growth of Hyundai Motors Group, as well as other automotive customers. The plant is expected to ramp up production in 2020 and also allows for further expansion.

## Mergers & Acquisitions

### Lanxess to sell organotin product line to PMC Group

November 13, 2019 — The European subsidiary of PMC Group N.A., Inc. (Mount Laurel, N.J.; [www.pmc-group.com](http://www.pmc-group.com)) will acquire the organotin specialties product line from the Organometallics business of Lanxess AG (Cologne, Germany; [www.lanxess.com](http://www.lanxess.com)). The acquired business includes Lanxess' global organotin catalyst, organotin specialties and intermediates product lines.

## LINEUP

AIR LIQUIDE
ALPEK
ALTIVIA
AVANTIUM
DAELIM
DOW
EVONIK
FIRMENICH
HEXION
KRATON
LANXESS
LINDE
LOTTE CHEMICAL
MCDERMOTT
PERSTORP
PMC GROUP
SAINT-GOBAIN
SHOWA DENKO
TEIJIN ARAMID
UMICORE
VERSALIS
WACKER



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**Firmenich acquires Evonik's CO<sub>2</sub>-extraction business**

November 6, 2019 — Firmenich (Geneva, Switzerland; [www.firmenich.com](http://www.firmenich.com)) has acquired the CO<sub>2</sub>-extraction business of Evonik Industries AG (Essen, Germany; [www.evonik.com](http://www.evonik.com)). This acquisition, which includes Evonik's facility in Trostberg, Germany, significantly expands Firmenich's capabilities in supercritical fluid extraction of natural botanical molecules for fragrance and flavor applications.

**Saint-Gobain to divest its French expanded polystyrene business**

November 5, 2019 — Saint-Gobain (Courbevoie, France; [www.saint-gobain.com](http://www.saint-gobain.com)), through its French subsidiary Placoplatre, has reached an agreement with Hirsch Servo Group and BEWiSynbra Group to sell its expanded polystyrene (EPS) business in France. The French EPS business has six industrial sites with around 240 employees and generated sales of around €70 million in 2018.

**Air Liquide acquires large industrial-gas business in Malaysia**

November 5, 2019 — Air Liquide (Paris, France; [www.airliquide.com](http://www.airliquide.com)) announced the acquisition of Southern Industrial Gases Sdn Bhd. (SIGSB), which is one of the key industrial-gas players in the Malaysian market. The company generates approximately €20 million in revenue annually and operates eight manufacturing and refilling facilities across Malaysia.

**Altivia completes acquisition of Dow's acetone-derivatives business**

November 4, 2019 — Altivia Ketones & Additives, LLC (Houston, Tex.; [www.altivia.com](http://www.altivia.com)), an affiliate of Altivia Petrochemicals, announced that it acquired Dow's Acetone Derivatives business and associated chemical manufacturing assets at Institute, W.Va., as well as the Institute Industrial Park. The Acetone Derivatives business manufactures ketones and carbinols, used primarily in the coatings, adhesives and pharmaceutical industries. It is the largest North American production facility of its kind.

**Kraton to sell its Cariflex polyisoprene business to Daelim**

October 30, 2019 — Kraton Corp. (Houston; [www.kraton.com](http://www.kraton.com)) has agreed to sell its Cariflex polyisoprene-latex business to Daelim Industrial Co. (Seoul, South Korea; [www.daelim.co.kr](http://www.daelim.co.kr)) for a purchase price of \$530 million. The transaction is expected to close in the first quarter of 2020.

**Alpek to acquire Lotte PET plant in the U.K.**

October 30, 2019 — Alpek S.A.B. de C.V. (San Pedro Garza Garcia, Mexico; [www.alpek.com](http://www.alpek.com)) announced that one of its subsidiaries has signed an agreement with Lotte Chemical Corp. (Seoul, South Korea; [www.lottechem.com](http://www.lottechem.com)) to acquire a 100% stake in Lotte Chemical U.K. Ltd., which owns and operates a 350,000-m.t./yr polyethylene terephthalate (PET) facility in Wilton, U.K. ■

*Mary Page Bailey*



## Workforce 4.0:

# The Human Side of Digital Transformation

As chemical process industries (CPI) companies continue to experiment with, invest in, and implement a host of digitalization tools, workforce engagement and involvement is the key determinant of success

**C**hemical process industries (CPI) companies are entering a critical stage in the movement toward digitalization (Industry 4.0), in which the majority of organizations are now initiating pilot projects aimed at improving operations with advanced digital tools. This includes a wide range of technologies, including data analytics, cloud computing, machine learning, artificial intelligence and many others. As the digitalization transformation of the CPI gains momentum, it has become clear that the movement is as much about people as it is about technology. The acceptance and involvement of workers is critical to the successful adoption and expansion of digital tools, as they are asked to adapt to new work practices.

Greg Smith, a senior consultant at the Cutter Consortium (Arlington, Mass.; [www.cutter.com](http://www.cutter.com)) who has worked with companies from across many industries on digital transformation initiatives, says “What I’ve found is that you can always make the technology work, but the ultimate success or failure of a digital initiative is always tied to the people.” He emphasizes: “Companies don’t adopt new technologies; people do.”

### Culture of adoption

The CPI has entered a critical stage in its evolution, where most companies are experimenting with the implementation of digital technologies, and are increasingly running pilot projects to determine how best to utilize them. In doing so, organizations are grappling with the reception of those new technologies by the workers who will have to use them, and are finding ways to engineer how the new technologies are incorporated by ex-



Quartec

isting personnel. Smith talks about creating the right culture for adoption, an approach his company calls “adoption engineering.”

“We tend to assume that humans will behave rationally, but that is only sometimes true,” Smith says. “Workers’ previous experiences, along with a large set of preconceptions, existing biases, heuristics, shortcuts, and so on, all color their view of a new technology and affect how they will receive it,” Smith says. The objective for companies then becomes how to create conditions that will motivate employees to embrace the technology.

Resistance to the introduction of new digital technologies can come from different sources. Some workers are threatened by change itself, and are not inclined to do something new, even if benefits are possible. Others resist externally imposed changes.

Additionally and importantly, resistance comes from a conception persistent among many workers that digital tools will make them less valuable to their organization. “The biggest hurdle we see is that workers have a lot of fear that digital technologies will result in job loss,” says Jane Arnold, global lead for process control technology at Covestro AG (Leverkusen, Germany; [www.covestro.com](http://www.covestro.com)).

## IN BRIEF

CULTURE OF ADOPTION

EMPLOYEE  
ENGAGEMENT

EXPERIENTIAL LEARNING

INDUSTRY-ACADEMIC  
PARTNERSHIP

But Arnold says the reality is different, and she's not alone. She and others view digitalization as an opportunity to liberate workers to undertake more valuable, higher-level functions that involve more creativity and imagination.

"Digitalization offers a way to change the way we work; the intent is not to reduce headcount," she says. "We have to maintain the human element in CPI operations. There are important differences between chemical processing and repetitive discrete manufacturing. The CPI needs many engineering, maintenance, operations and other functions that will not be eliminated by digital tools."

Michael Risse, vice president for advanced analytics software provider Seeq Corp. (Seattle, Wash.; [www.seeq.com](http://www.seeq.com)) also sees concern on the part of some workers that digital technologies will replace job functions, but stresses that the fears may be overblown. "Digital technologies will enable workers to do things that haven't been possible before —

that's the defining experience with Seeq. Applications reduce the time required for certain tasks so workers can devote time and intellectual resources to areas that could be extremely valuable to the company, but that in the past, were not addressed because people were devoting their attention to routine operations."

The idea that digital tools are a liberating force for workers in the CPI is also shared by Rajiv Anand, CEO of Quartic (Oakville, Ont.; [www.quartic.ai](http://www.quartic.ai)), a provider of artificial intelligence solutions for the minerals, chemicals, petrochemicals, pharmaceuticals and food and beverage industries. "Artificial intelligence (AI) and machine learning allow engineers to move toward more proactive analytics, rather than simply investigative, root-cause analysis work," he says, adding that this results in workers having a more visible impact of their work sooner.

AI with machine learning tools also allow engineers to "zoom out," Anand says, by which he means looking at the interactions within a process at the level

of a unit operation or at the full plant, rather than at an asset or loop level. "This is particularly useful for processes that have a lot of inherent lag and are highly interactive," Anand notes.

Taking the idea of digital's freeing quality further, Covestro's Arnold views digitalization as a continuous improvement exercise. "If you are able to solve one problem by using digital tools, you free up personnel to work on the next problem that would have just been neglected, or tolerated or ignored. "People add value; so we need to utilize them," she says.

Duane Dickson, vice chairman and U.S. Oil, Gas & Chemicals leader, Deloitte LLP (New York, N.Y.; [www.deloitte.com](http://www.deloitte.com)) says an ideal model would be to have digital tools deployed to help people do their jobs more safely, faster and more efficiently, then utilize the surplus person-hours for solving commercial and technical problems that companies don't normally have time to address because they are devoting all resources to producing products. "This scenario does happen," he says.

### Employee engagement

In addition to overcoming fears, the adoption and overall success of digital tools also depends on the engagement and involvement of employees with the development of the digital solutions themselves. "Nothing will be adopted by end users unless they are involved in developing the solutions," says Covestro's Arnold.

Covestro recently began a pilot project at a site in China (Caojing Chemical Works) with applied artificial intelligence (AI), where the company uses machine learning software to recognize patterns and deviations and to predict equipment failure up to eight months in advance, and avoid unscheduled downtime. "The project is about AI, but just as much, it's about how to get employee engagement right, because without employee engagement, no digital technologies will work," Arnold says.

The pilot project is beginning with 20 volunteers representing all different functions within the plant, including maintenance, operations, plant manager, and so on. The team is working on revising work practices and

building a library of information that employees can use to quickly assess the health of an asset. “We need to figure out what makes a system intuitive for workers. What do they like? What would make their work easier, faster or better? What are their pain points?” Arnold says, adding “We want to help them, not just give them another screen to look at.”

This approach allows each site, plant, unit and team to customize the digital solution to allow for nuances that differ from the others — different ‘personalities,’” Arnold says.

Cutter’s Smith says the way to undertake smart digital transitions is to give workers freedom to try different things and quit the things that don’t work. A corporate culture where “failure is not an option,” does not help in digital transformations; it only hinders.

Smith remarks that engineering-driven companies and science-based industries sometimes have a hard time adopting digital technologies because it often requires them to give up some hierarchical control. “Companies need to start small, generate some validated data, then make incremental changes. They need to involve their workers in those incremental changes, and in doing that, will have to embrace a messier distribution of authority than they are generally used to,” he says.

Another aspect of engaging employees in the development of digital solutions comes from the deployment of machine learning algorithms. Quartic is looking to overcome that lack of trust that occurs when AI models are built by one group and used by another. “Most of the digital transformation in this [AI] context is led by IT [information technology] and data science people,” Quartic’s Anand says, which is a large barrier. When this happens, machine learning algorithms can appear to be a “‘magical black box’ that is doing something we don’t understand, and therefore, we don’t know if we should trust the predictions,” Anand says.

The best way to overcome this is to let those who will be impacted by the technology build the AI models. The tools have to be built for that workforce so they can develop their own AI applications, argues Anand. Fur-

ther, employees should not be forced to learn new tools or techniques — instead the new tools should become a natural part of their workflow.”

Quartic provides a platform that enables process manufacturing subject matter experts to build intelligence with their own knowledge, and with tools that look and feel like the operational technology (OT) systems that they are already familiar with, Anand says.

### Experiential learning

In 1983, the British psychologist and scholar Lisanne Bainbridge outlined the “ironies of automation,” in a paper that argued that while highly automated systems may require less human input overall, the interaction with the system that humans do have becomes more important. Although the idea predates the use of advanced digital tools and AI industrially, it still has traction in some contexts.

Don Glaser, CEO of Simulation Solutions Inc. (Shrewsbury, N.J.; [www.simulation-solutions.com](http://www.simulation-solutions.com)) mentions Bainbridge’s work when he remarks that among the challenges associated with digital transformation are that, as the level of automation increases, the actions required of humans become more consequential, and the skills and practice of workers becomes more important.

When process operators and engineers are younger and less experienced, they are less well equipped to respond appropriately when a process upset occurs and the automation tools break down, Glaser says. At some point, people will have to manually intervene to break the automation loop, but if they haven’t practiced, they don’t have confidence in manipulating the process, he adds.

Becoming more reliant on digital tools can sap humans of process knowledge, but digital tools can also help solve this issue. Duane Dickson at Deloitte says that part of the solution is to increase hands-on learning. Companies need to make digital technologies more accessible, so that employees have opportunities to play around with the tools offline, and get familiar with how they work and how they interact with the process. “The more familiar they are, the



more likely they will be to give buy-in for the implementation,” he says.

In an example of experiential training, Don Glaser’s company Simulation Solutions offers “active learning environments” designed to provide simulator-based training that fills gaps in hands-on learning. “Chances for experiential learning are lacking at all levels — operators, engineers, supervisors,” Glaser says. “For young engineers, there is an operational sense that is insufficient, and the biggest gap is in experiential learning.” Workers need to understand how processes work, so they can intervene when the automation fails.

“Simulations are designed to ‘de-instrument’ the process, so workers get a better idea of what the automa-

tion is designed to do,” Glaser says. Works. Among the outcomes of the partnership was The Center for Petrochemical Energy and Technology (CPET) at SJC, which was opened in August 2019, with 29 custom laboratories (six more are still being built). CPET is designed to foster hands-on learning, as well as for exploring ways to leverage digital tools to change curriculum, content, evaluation and more, says SJC associate vice chancellor Jim Griffin.

CPET has enjoyed close collaboration with equipment companies and operator companies since its inception, Griffin notes, citing an example in which operations personnel and trainers from LyondellBasell (Rotterdam, the Netherlands; [www.lyondellbasell.com](http://www.lyondellbasell.com)) came to the school to work with students on dis-

tributed control systems, and in how to look at data and make decisions about dealing with different process scenarios. Griffin says representatives from other CPI companies have worked with students on mobile digital field devices, wireless transmitters, making decisions with trending data, digital alarm management and other topics, and Emerson Automation Solutions has provided automation equipment to the center’s fully functioning glycol-processing unit.

“We are continually looking to add capabilities to use AI to improve teaching and learning,” Griffin says.

Bozic, Glaser and Garvey led a competition recently at the AIChE fall meeting in Orlando, where teams of students from different universities competed against each other in a knockout tournament format. “After the in-class competition, we take time for after-action review,” Bozic says, “which forces students to reflect on how the process engineer responded to issues and what actions they took.”

Other examples of gamification include scenario plays, in which a machine-learning model is built and then presented with data for different scenarios and the outcomes observed, Quartic’s Anand says. “For engineers and technical people in the CPI and other process industries, gamification has to be done in context. Scenario plays is one of the most useful ones that we have experienced.”

Competition also works. “We do reverse hackathons — where an AI model is built by an expert, but you then challenge the peers to improve it or “crash it” based on their knowledge of the subject,” Anand says.

Cutter’s Smith told of another example where a water utilities organization created a “treasure hunt” for finding unknown missing legacy corporate assets (old underground piping systems) using digital tools. ■

*Scott Jenkins*

**Editor’s note:** For more on workforce issues of the digital transformation, see the online version of this article at [www.chemengonline.com](http://www.chemengonline.com)

***“Digitalization offers a way to change the way we work; the intent is not to reduce headcount,”***  
***—Covestro’s Jane Arnold***

tribution is designed to do,” Glaser says.

Another example related to hands-on training appeared in September, when Emerson (St. Louis, Mo.; [www.emerson.com](http://www.emerson.com)) introduced its Performance Learning Platform, a portable and compact automation-technology training solution that enables hands-on training to prepare workers to maintain plants safely and efficiently. The platform reinforces competencies essential to fostering digital transformation and helps close the workforce skills gap, Emerson says.

### **Industry-academic partnership**

Industry-academic partnerships are proliferating to fill in some of the gaps in experiential learning as well, both to train students in using digital tools, but also in using digital tools to train students on conventional process equipment. An example of this can be found at a center opened this autumn at San Jacinto College (SJC; Pasadena, Tex.; [www.sjcd.edu](http://www.sjcd.edu)), a school located in the Houston ship channel, home to dozens of CPI plants.

In 2015, the East Harris County Manufacturer’s Association developed an initiative for realizing a vision of an enhanced workforce for process plants called PetroChem

Work. Among the outcomes of the partnership was The Center for Petrochemical Energy and Technology (CPET) at SJC, which was opened in August 2019, with 29 custom laboratories (six more are still being built). CPET is designed to foster hands-on learning, as well as for exploring ways to leverage digital tools to change curriculum, content, evaluation and more, says SJC associate vice chancellor Jim Griffin.

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### **Gamification of learning**

In another industry-university collaboration designed to provide realistic training, Columbia University (New York, N.Y.; [www.columbia.edu](http://www.columbia.edu)) professor Robert G. Bozic is working with Simulation Solutions chief engineer Matt Garvey and CEO Don Glaser on a simulated process safety exercise that has been “gamified,” a concept that refers to the application of elements from video gaming into work, training and education tasks.

Bozic and Simulation Solutions have developed a competition called ChemE-Sports, in which chemical

# The Changing Face of Simulation

Easier-to-use features and simplified integration lead to new applications for simulation software

## IN BRIEF

### SIMPLIFYING SIMULATION

SMALLER, BUT  
IMPORTANT  
CHALLENGES

REDUCING RISKS

SUSTAINABILITY

MAINTENANCE

TRAINING

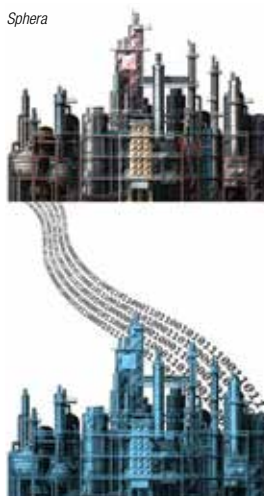
THE FUTURE

Simulation software and its capabilities have come a long way in recent years. The latest versions include easier-to-use and more advanced features, increased computing speeds and simplified integration with other simulation programs, as well as data analytics and Industry 4.0 technologies. These modern features allow today's simulation tools to be employed in a variety of applications throughout the lifecycle of a plant. As a result, chemical processors are using simulation not only for design and optimization tasks, but also for other challenges, such as increasing safety and avoiding operational risk, achieving sustainability goals and training employees.

### Simplifying simulation

While simulation has become the de facto method for designing and optimizing processes in the chemical process industries (CPI), for many years, users didn't apply the technology to other types of analysis, such as overall profitability, safety issues or smaller engineering problems, because it took too long to get an answer or because the simulators were too difficult to set up and use. As a result, some software providers have built solutions with lower-fidelity models that are easier to build and use. Meanwhile, other providers have taken steps to increase speed of calculations and simplify the use of rigorous process simulators.

"Democratization of simulation software is becoming more important," says Steve Brown, CEO of Chemstations (Houston; [www.chemstations.com](http://www.chemstations.com)). "Everyone in the organization should be familiar with and use simulation to address challenges, but we find there's resistance to doing that, so the



**FIGURE 1.** Sphera Operational Risk Management Digital Twin software brings together the data collected from enterprise systems, mobile applications, sensors and human-derived inputs as part of an industrial internet of things (IIoT) strategy to produce a computer-generated risk map

expertise tends to get siloed into a few experts. But to get maximum value from the simulator and the answers it can provide, you need to provide more people with the ability to use the simulator and its data, and the way to do that is to make it easier to use."

As a result, simulation providers have focused on making the latest versions more user friendly. "We have reduced the number of mouse clicks needed to get to where you need to go, increased visibility of the most used functions and provided really good graphical interfaces with better reporting capabilities. This allows engineers to more easily use the simulator to solve a problem and take the data out of the simulator to present the results to the people who need to use it to make decisions."

Another change Chemstations has made is to increase the computing speed of its rigorous process simulator by taking advantage of parallel processing, which uses all available computing cores. "This means that instead of using just one core of the user's computer, we can spread the workload across as many cores as are available, which will speed the process considerably," explains Brown. While the initial intent of the improved calculation time was to allow faster execution of large optimization projects, the increased speed opens the door for simulation of smaller-scale projects and "what-if" studies.

Because newer simulation programs are easier to use, says Brown, it allows more collaboration between departments. "In the past there were silos of information where

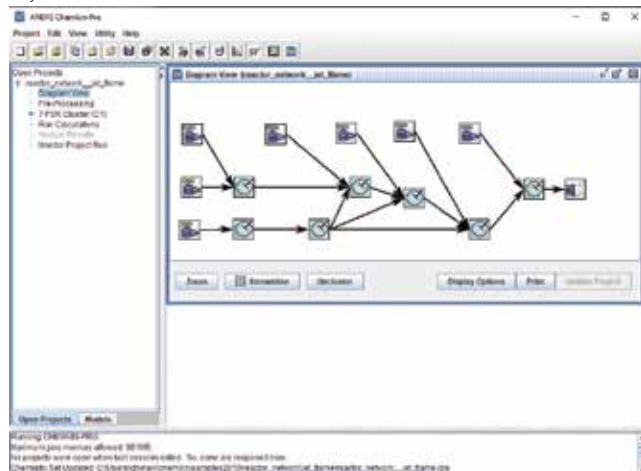
one group used a set of tools and generated data, then passed it to the next group,” he says. “But it makes more sense for these separate groups, who are really all working to achieve the same goals, to use the same simulation model and data. Sharing the model means all the data is consistent, so we are working toward making sure the data from the simulator can easily export into the data standards that exist within other engineering tools.”

For example, an engineering team may build a model and then wrap an Excel interface around it or send the data to the supervisory control and data acquisition (SCADA) system so that operations and maintenance staff can see what’s going on and perform their own engineering studies without having to understand the underlying engineering of simulation or be trained on the simulator. “The way this type of integration works is that the engineer builds a model, connects it to the OPC [open plat-

form communications], and the operations and maintenance staff can see the values coming from the simulator and apply them to performance monitoring and other tasks,” explains Brown.

Scott Lehmann, vice president of operational risk with Sphera (Chicago, Ill.; [www.sphera.com](http://www.sphera.com)) agrees that simulation and the plant’s digital twin can be used to pull all the disparate systems together for a better view. “There are a lot of different systems managing separate things, so facilities often have disparate data, systems and business processes, which means there are a lot of separate de-

cisions being made and, often, they are being made out of context,” says Lehmann. “The digital twin starts to pull it together with dynamic visualization so users can see the geography view — here’s the status of the plant, here are the various impairments, here are the activities that are hap-



**FIGURE 2.** Easier-to-use simulation systems with advanced capabilities increase the ability of simulators to address a variety of challenges. Here, Reactor Network mimics combustion of a gaseous jet flame in ANSYS Chemkin-Pro to efficiently predict emissions





**FIGURE 3.** With sustainability as a goal, processors are considering things like reducing energy use and greenhouse gases as an important metric to watch. Simulation can help them examine different ways to significantly reduce energy use and greenhouse gas emissions and how doing so will affect productivity and profitability both for new processes and existing ones

pening. By pulling all this together, it provides a richer view, making it easier to make informed decisions.”

And, as we enter the realm of Industry 4.0, integration becomes more important than ever, says Ahmad Haidari, global industry director, process, energy and power with Ansys (Canonsburg, Pa.; [www.ansys.com](http://www.ansys.com)). “When we talk about plant and asset performance, we often think of data analytics, which includes collecting data from sensors and historical behavior and placing it into the data analytical platform to be reviewed, so now the question becomes, ‘What role will simulation play in Industry 4.0?’” he says. “The answer lies in the digital twin. Users can model an existing asset, merge it with sensor data, operational data and historical data and effectively marry engineering and operations with a virtual replica of the plant that can be employed to solve real-life issues.”

Haidari provides an example: If you’re looking at the performance of a mixing tank and the sensors show

analytics and simulation allows simulation-based digital twins to help companies see the reason why something is happening with the performance of equipment and solve the problem in a more informed manner, allowing them to better control the equipment and process, prevent unwanted downtime, reduce waste and predict when a process may go out of control.”

### Smaller, but important challenges

Thanks to easier-to-use simulators, smaller challenges can now be addressed, and one of the newest applications for the technology falls under increasing safety and mitigating operational risks. When the simulation program has the ability to take data generated from the assets, the historian, operator rounds or the maintenance management system, it can be used to monitor assets in real time through a dynamic visualization. This allows users to simulate “what-if” scenarios without impacting the live plant, which can be extremely helpful when it comes to

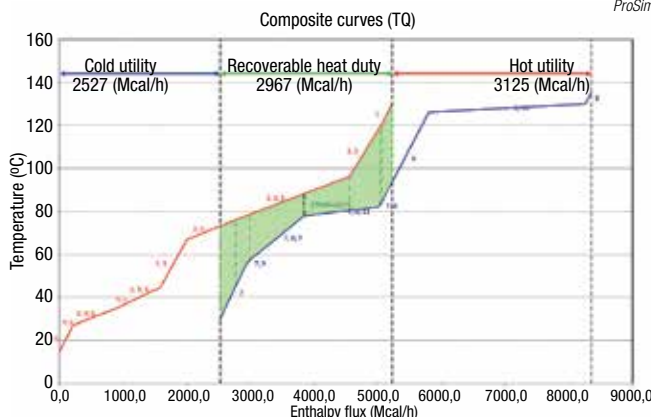
the material being mixed is too thin, you may not know why, but the digital twin of the same mixing tank shows the material is too thin because the shear rate is too high, so the solution is to back off the impeller. “Tight integration between data an-

to play with different scenarios so they understand the risks of various scenarios and the trade-offs of each action and risk and then take the path that best suits their needs,” Sphera’s Lehmann says. “It provides actual insight that allows them to make informed decisions about whether they need to execute changes, when and where they need to execute them and which actions will result in the least amount of risk,” (Figure 1).

Lehmann continues: “The value of the digital twin in this type of risk management is that it makes the hazards and risks visible and available in real time so users can connect process safety management to operations and balance the risks against productivity.”

An example would be an operator who is about to open a vessel, but instead of going in uninformed, he may use integrated information from the simulator studies to better understand the current state of the plant, the current state of that vessel and how those factors may impact his safety and the job he’s about to do, as well as how opening that vessel may impact productivity of the vessel itself and the entire plant. “The concept behind using simulation for operational risk management is that it provides transparency and allows processors to balance risk against productivity,” says Lehmann. “Is this the right time to open the vessel? Will it stop production and cause a problem with productivity or safety? Is it better to wait and do it later or will waiting create a failure situation where productivity may be more drastically impacted down the road? It’s not a case of doing nothing, it’s a case of getting that balance right.”

Avoiding safety risks is another benefit of simulation tools, says Ansys’s Haidari. “Industry is pushing operational boundaries in order to increase efficiency, but this means processes are working to extremes and operating conditions now involve higher pressures and higher temperatures, which can lead to accidents,” he says. “But, via simulation models, processors can explore and determine under what conditions a reactor may veer into thermal runaway or



**FIGURE 4.** Simulis Pinch allows any engineer to easily apply the pinch technology to find the best possible energy exchanges between streams to be heated and streams to be cooled

looking at the risk profile of certain tasks or actions and finding ways to offset or mitigate that risk.

### Reducing risks.

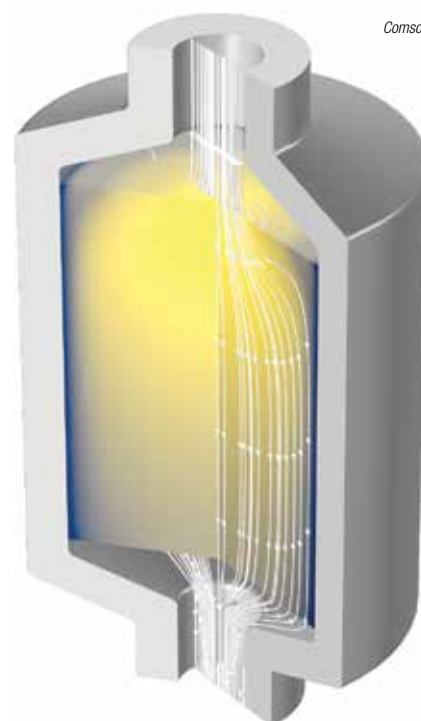
“Using simulation to see the operational risks and how they come together to impact the cumulative risk allows users to examine risk data in real time,

face equipment failure due to corrosion or erosion. The models can tell us how to safely and efficiently run the reaction without unwanted by-products, thermal runaways or hazardous leaks" (Figure 2).

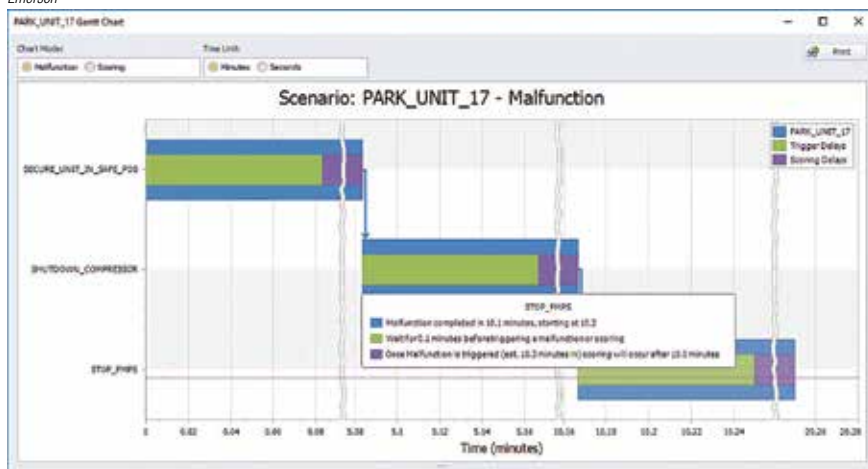
**Sustainability.** Simulation is also being applied toward improving sustainability throughout the plant, according to the experts. "Simulators have always been very good at modeling the steps necessary to clean up the process, allowing users to model carbon capture, scrubbing of contaminants, wastewater clean up and other necessary processes, but companies didn't use it," says Paige Marie Morse, industry marketing director, chemicals, with AspenTech (Bedford, Mass.: [www.aspentech.com](http://www.aspentech.com)). "But now that sustainability is becoming a goal, people are considering things like reducing energy use and greenhouse gas emissions as important metrics to watch and simulation can help them examine different ways to significantly reduce energy use and greenhouse gas emissions and how

doing so will affect productivity and profitability both for new processes and existing ones" (Figure 3).

Olivier Baudouin, process manager with ProSim (Labege, France; [www.prosim.net](http://www.prosim.net)) agrees. "Different simulation tools can be used to address a variety of sustainability issues, including energy use and water treatment," he says. "For example, our Pinch Analysis can be used to optimize the thermal power consumption and, coupled with our Exergy Analysis, improve the energy efficiency of a process. And, our Water Pinch analysis module can be integrated into simulation software to reduce water consumption and wastewater generation, linked with useful unit operation models for water treatment, such as ultra-filtration, nano-filtration and reverse osmosis. Of course, at the end, the profitability of the plant will lead to the selection of the technological choices, thus a powerful economic evaluation module has to be available in simulation software, allowing users to find the balance



**FIGURE 5.** The latest version Comsol Multiphysics provides an entirely new sketching tool for easier creation and more versatile parametric control of geometry models



**FIGURE 6.** A new release of Emerson's Mimic makes it easier for plants to develop a more accurate digital twin

between sustainability and profitability," he says (Figure 4).

**Maintenance.** Maintenance is another area that can now take advantage of simulation and its ability to directly connect to the process, says Ed Fontes, chief technical officer with Comsol (Stolckholm, Sweden; [www.comsol.com](http://www.comsol.com)). "Once connected to the process, the model is not generic, rather it's a detailed replica of the specific process, making it possible to monitor and plan maintenance of a reactor, process or plant," he says. "Following equipment, such as a reactor, with a connected simulator will allow you to see what is happening with that reactor in a more useful way than just using measurements or a digital twin alone. Integration of the two has led to the practice of running large processes with very few engineers because everything is optimized and controlled using models and sensors instead of having employees looking at individual displays. Everything is centrally connected to the computer systems, which are connected to the model allowing users to see what all that data means for the process and maintenance of the reactor" (Figure 5).

He continues: "The digital twin of the plant or of the different units within the plant can even be run in advance of the actual process so that the process can be watched in detail and users can estimate when the equipment will be subjected to fatigue or failure and take maintenance action before that happens. Or, you can know in advance when there will be

deactivation of the catalyst and know how much time you have before you have to change or regenerate it. Connected simulation allows you to do these maintenance tasks with greater accuracy by continuously monitoring the equipment, process and plant with simulation and sensor measurements to provide a detailed view of what will happen and prevent shutdowns before they occur."

**Training.** Simulations of the control systems can also be helpful for training operators. "In the past, the digital twin was used to train panel operators and provide that plant interface with the offline control system environment, but now, using pre-developed 3D CAD [computer-aided design] drawings and software tools that automatically generate the 3D environment, it provides a very high-resolution, high-quality virtual-reality view of the plant, allowing users to bring field operators into the same environment," says Mart Berutti, vice president of process simulation with Emerson (Austin, Tex.; [www.emerson.com](http://www.emerson.com)). "This means that without even having the plant built, users can have a virtual control room with a control system simulator with a panel operator in there interacting with the control system in a high-fidelity simulation of the process. Field operators can be working in the same virtual environment doing simulated field routes. The cost basis of this solution has come down drastically and the time to build it has also been reduced, so it's a cost- and time-effective way to get operators trained on a

new asset before it is even built and operating" (Figure 6).

Amanda Thompson, SIMIT product marketing manager, USA, with Siemens (Plano, Tex.; [www.siemens.com](http://www.siemens.com)) agrees that control-system simulators are advancing training. "It provides the opportunity for extremely realistic operator training because the operator training system is based on the same control system they will use in the real plant," she says. "It shows the same operator screens so they learn how to navigate through them. They can address alarms and work different operator procedures all in the same environment they would use in the real plant, but without the risk of performing training in a real plant situation where a training error could result in negative impacts to the process or safety. Simulation allows them to redo the operating procedure over and over until they learn how to do it correctly."

## The future

And, experts say that due to the easier-to-use features and ability to integrate simulation with other programs, the list of useful applications will continue to grow in the future. "In reality, everything can't be measured and everything can't be simulated, so the real crux of the issue is how can I use what can be measured and what can be simulated in a hybrid fashion," asks Ravindra Aglave, director, energy and process/computational fluid and particle dynamics, simulation and test services, with Siemens. "The problems processors face are complex and can't be solved via one single software platform. Instead, it is a portfolio containing many different softwares, each intended for a specific engineering aspect of the chemical process. These softwares have all existed for decades, but with today's outlook on digitalization and having a digital thread throughout the lifecycle of the plant, more and more software platforms are becoming integrated and compatible, allowing processors to work in a co-simulation environment which can plug results from one study into the next and so on for all kinds of improvement opportunities in the future." ■

Joy LePree

# Focus on Valves

Rembe



## Safe combustible-dust-explosion isolation

Isolation is essential to protect adjoining system components against the spread of combustible dust explosions. Tanks, silos, dust collectors and other equipment are usually connected by pipelines through which, if an explosion occurs, fire and pressure spread very rapidly. In addition, the intensity of the explosion in connected containers is increased by pressure piling and flame jet ignition. This sequence of events can be prevented by the EXKOP isolation system, consisting of a control panel and one or more quench valves (photo). The integrated elastomer seal within the quench valve closes within a few milliseconds, triggered by a signal from an Explosion Panel, a Q-Rohr, Q-Box, an infrared signal or pressure/temperature sensors. — *Rembe Inc., Charlotte, N.C.*

[www.rembe.us](http://www.rembe.us)



## More control for this electric valve actuator

This company has increased the versatility of the CK range of modular electric valve actuators with the introduction of the CK Atronik (photo), an intermediate-level integral control option, providing a ready-to-operate actuation solution to meet the standard requirements of many plant specifications. The CK Atronik control module houses a reversing contactor starter with mechanical and electrical interlocking. Connection to a suitable power supply is all that is required for local operation of the actuator. Digital microprocessor-driven functionality delivers reliable motor control for isolating, regulating or modulating valve duties. Integral local-control selectors are provided, together with clear LED status indication of valve open, valve closed, valve moving and alarm. — *Rotork plc, Bath, U.K.*

[www.rotork.com](http://www.rotork.com)



GF Piping Systems



ITT Engineered Valves

## NSF lead-free valve family for commercial water applications

This company has introduced a family of NSF lead-free brass valves (photo) designed to handle high loads and

strong flowrates in commercial-grade and light-industrial water-distribution applications. Valve styles include pressure reducing, thermostatic balancing and thermostatic mixing. The compact, direct-acting Pressure Reducing Valves (PRV) Type 1319 and 1339 feature excellent control characteristics, even at low flow-rates. This patented design, which offers a 416 stainless-steel floating seat and modular construction, allows for a more compact size. The Type 6320 Thermostatic Balancing Valve regulates the flowrate in hot (up to 158°F) water circulating systems by continuously sensing the return water temperature with an integrated thermostat, ensuring consistent system temperature. The Thermostatic Mixing Valves Type 3409 and 3419 accurately deliver tempered water to hot-water-distribution systems. — *GF Piping Systems, Irvine, Calif.*

[www.gfps.com/us](http://www.gfps.com/us)

## This diaphragm valve touts reduced maintenance

The EnviZion valve (photo) has embedded technologies that allow for a more streamlined installation and maintenance process, delivering less downtime, longer preventative maintenance cycles and greater production capacity for manufacturers. An integrated thermal-compensation system provides a constant sealing force, helping to eliminate the effects of thermal cycling. The EnviZion diaphragm can withstand the wear of production cycles and maintains a reliable seal, minimizing the risk of leakage and batch contamination. The EnviZion valve delivers increased productivity by keeping operations online and running longer, as well as reduced operating costs yielding over 90% reduction in maintenance time, says the company. — *ITT Engineered Valves, Lancaster, Pa.*

[www.engvalves.com](http://www.engvalves.com)

## This actuator is lighter than its stainless-steel counterparts

Designed to operate at 4.5 bars while maintaining closure perfor-





mance of up to 10 bars at 100% pressure drop, the Saunders P345 compact polymer pneumatic actuator (photo) will simplify plant infrastructure and provide a lower total cost of ownership compared to existing technologies, according to the manufacturer. This performance is achieved within a highly compact dimensional envelope and

at a 30% lighter weight compared to typical stainless-steel variants, reducing dead-leg between associated valves. The use of polyamide housing and a stainless-steel bonnet provides a robust interface. Capable of withstanding temperatures between -10 and 100°C, the P345 is available in sizes DN8 (0.25 in.) to DN100 (4 in.) in spring-to-close, spring-to-open and double-acting modes of operation. — *Crane ChemPharma & Energy, a business of Crane Co., The Woodlands, Tex.*  
**[www.cranecpe.com](http://www.cranecpe.com)**

### **This ball valve now has a stem-position indicator disc**

This company recently introduced a new stem-position indicator disc for its Camseal metal-seated forged ball valves (photo) for easy, precise on-site identification and inspection of the open-close status of the valve. The high-quality severe-service valves are available in ½- through 4-in. sizes with socket weld, butt weld and flanged ends, in pressure classes from ASME



900 through 4500. The new Stem Position Indicator Disc design (patent pending) increases the visibility and accuracy of stem and ball alignment into the valve seat. This is critical in severe applications, such as steam, where positive, sustainable shutoff is critical. — *Conval, Enfield, Conn.*

**[www.conval.com](http://www.conval.com)**

Emerson



Val-Matic Valve & Manufacturing



Circor International



Gericke USA

### New manifold valve design for pressure transmitters

Manifolds shut off or equalize pressure at the transmitter, and also provide the critical mounting mechanisms required in many installations. The recently introduced Rosemount R305 Integral Manifolds and Rosemount R306 In-line Manifolds (photo) have been designed to offer significant user improvements on these basic functions. The most important improvement for both manifolds is the new Pressure-Lock Valve design, which simplifies high-pressure operation, increases safety and enhances reliability. New features include: a two-piece stem that does not rotate in the seat, providing solid closure with minimal wear; easier turning while delivering positive shut-off; an adjustable packing nut that simplifies valve maintenance; and back seating that prevents blowouts for increased user safety. The stem and bonnet threads are fully isolated from the process fluid to minimize potential corrosion, and modular packing ensures only the stem and body are exposed to the process fluid. — *Emerson, Shakopee, Minn.*  
[www.emerson.com](http://www.emerson.com)

### These butterfly valves are built for trouble-free operation

Used in thousands of field installations in municipal, industrial and power applications throughout the world, the American-BFV butterfly valves (photo) are highly engineered to provide long life and trouble-free performance. The ductile iron disc adds strength, allowing the disc to have a smaller cross-section and providing improved head-loss characteristics. Stainless-steel taper pins are designed to utilize tangential forces to provide the most secure method available for locking the disc to the shaft for strength and rigidity. — *Val-Matic Valve & Manufacturing Corp., Elmhurst, Ill.*  
[www.valmatic.com](http://www.valmatic.com)

### This control valve features a fail-safe function and more

The REflex Quick Change Seat (QCS) control valve with REact 30 DC-PoP smart actuator (photo) is a flexible all-in-one solution for noise reduction and high-pressure-drop applications. The REflex QCS control valve assembles and disassembles in four quick

steps without the need for special tools, accelerating maintenance by up to 85%, says the company. Tool-free seat exchange allows for quick adaptation to changing conditions. Featuring optimized high-capacity flow paths and interchangeable trim, the two-way REflex QCS control valve supports a variety of media and meets NACE standards for use with abrasive liquids and gases. All REflex valves are available either as ANSI or DIN size, ensuring that direct replacement is always possible. — *Circor International, Inc., Burlington, Mass.*  
[www.circor.com/rtk](http://www.circor.com/rtk)

### Automatically guard against product contamination

The RotaSafe valve-rotor protection system (photo) automatically detects contact between the rotor and housing and instantly shuts down power to the drive motor to prevent any metal-to-metal contact from contaminating the product and from damaging the valve components. Monitoring valve performance in 24/7 operation, the proprietary RotaSafe system responds instantly to contact due to product buildup, bearing failure, excessive load on the rotor and to other maintenance issues common to processing powders. Developed to safeguard food, beverage, chemical, pharmaceutical, plastic and other materials where purity is paramount, the RotaSafe rotor-contact monitoring system is included as standard equipment on the company's Rotaval line of rotary valves. The line of rotary valves comprises the food-grade Hygienic Series valves, the versatile Heavy-Duty Series, the Extra Heavy-Duty Series for highly abrasive and extreme situations, and custom valves for unique applications. — *Gericke USA, Inc., Somerset, N.J.*  
[www.gerickegroup.com](http://www.gerickegroup.com)

### Electronic expansion valves with 6–8-ton cooling capacities

This company recently expanded its family of Modular Silicon expansion valves (MSEV; photo) to include cooling capacities of 6, 7 and 8 tons (R-410a). The MSEV is an electronically controlled, normally closed and one-directional flow valve. It can be used for refrigerant mass-flow control in industry-standard HVAC (heat, ventilation and air conditioning) and refrigeration systems. The MSEV provides



precise superheat control and quick mass-flow adjustments through a closed-loop control methodology achieved with the company's Universal SuperHeat Controller (USHC). Embedded with the newest generation of MEMS chip, silQflo Silicon Servo Valve (SSV), the MSEV is said to be the fastest-responding refrigerant expansion valve in the industry. — *DunAn Microstaq, Inc., Austin, Tex.*  
[www.dmq-us.com](http://www.dmq-us.com)

#### **Combined pulsation damping with a backpressure valve**

In July, this company received U.S. Patent 10,353,409 for its Hybrid Valve (photo), said to be the world's first combination pulsation dampener and backpressure valve. The Hybrid Valve combines the steady flow control of a pulsation dampener and the regulation of a backpressure valve to deliver the performance and functionality of both in a single piece



of equipment. In a metering pump system, using a back pressure valve alone does nothing to improve fluid flow. When put in series with a pulsation dampener, the flow improves significantly but, according to company performance tests, results do not match the performance of the single-construction Hybrid Valve for the steadiest flow. Further, as a single unit, the Hybrid Valve takes up less space and has fewer leak points for improved functionality and lower maintenance costs. — *Blacoh Industries, Riverside, Calif.*

[www.blacoh.com](http://www.blacoh.com)

#### **Miniature solenoid valve offers high flow, low power and more**

This new generation of three-port solenoid valves offers the combi-



nation of high flowrates, low leakage and low power consumption in a miniature 10-mm package. The genvi solenoid valve (photo) is capable of achieving minimum flowrates of 30 to 40 std. L/min at 15 psid and its spike-and-hold profile results in ultra-low power consumption (318 mW) during continuous-duty operation on air and compatible gas applications. This reduces system-level heating and improves battery life, making it suitable for applications with challenging power budgets. In addition, genvi valves are designed to provide response times of less than 10 ms in applications with an operating temperatures ranging from 40 to 120°F. Typical applications for the valves include molecular diagnostics, oxygen delivery, environmental monitors, compression therapy, breath analyzers or wherever high flow and low power cannot be sacrificed for size and reliability. — *Lee Products Ltd., Gerrards Cross, Buckinghamshire, U.K.*

[www.leeproducts.co.uk](http://www.leeproducts.co.uk)



Alfa Laval Kolding



High Pressure Equipment



GEMÜ

### Fluoroelastomers enhance the performance of valves

Components used in industrial equipment must withstand taxing conditions in order to reduce downtime needed to repair or replace malfunctioning parts. To help manufacturers of industrial parts address this challenge, this company offers Aflas 100 Series fluoroelastomers to enhance the performance and extend the life of pumps, seals and valves used in a variety of harsh processing applications. Aflas fluoroelastomers are resistant to acids, bases, solvents, hydrocarbons, sour oil and amines, as well as extreme temperature ranges and high-pressure environments. Aflas 150P, 100S and 100H are FDA-approved for food contact. — *AGC Chemicals Americas Inc., Exton, Pa.*

[www.agcchem.com](http://www.agcchem.com)

### Mixproof valve for aseptic applications

This company recently introduced an aseptic double-seat valve to its range of mixproof valves. The new Aseptic Mixproof Valve for sterile process applications (photo) is based on the same modular architecture as the aseptic version of the company's Single Seat Valve (SSV), and is said to reduce the total cost of ownership for dairy, food, beverage and other manufacturers by up to 45% compared to the leading aseptic double-seat mixproof valves. Initially, the Aseptic Mixproof Valve range will include these valve sizes, which meet most manufacturer requirements: ISO 51 mm (2 in.), 63.5 mm (2.5 in.) and 76.1 mm (3 in.). The optimized design of the Aseptic Mixproof Valve makes cleaning and sterilization easier, thereby enabling more production uptime. With a highly flushable design and no domes in the product and steam areas, the valve provides better cleaning capabilities than other double-seat aseptic mixproof valves. — *Alfa Laval Kolding A/S, Denmark*

[www.alfalaval.com](http://www.alfalaval.com)

### New valves sizes for very-high-pressure applications

Earlier this year, this company introduced new sizes to its family of ultra-high-pressure valves, fittings and

tubing. The company added 3/8 in. and 9/16 in. O.D. valves and fittings (photo) designed to ensure safe and easy plumbing for pressures up to 100,000 psi. The new sizes of valves are available in four body styles: two-way straight, two-way angle, three-way/two inlets and three-way/one inlet. Accompanying fittings include check valves, elbows, tees and crosses. The new valves feature 316 stainless-steel high-tensile bodies, non-rotating stem tips to ensure a long life on valve seats, packing below the stem threads and a positive gland-locking device. — *High Pressure Equipment Co., a subsidiary of Graco Inc., Erie, Pa.*

[www.highpressure.com](http://www.highpressure.com)

### These anti-siphon valves are corrosion resistant

Used mainly to prevent gravity-induced siphonage from storage tanks, the Series RVDT remains closed under the pressure created by the presence of liquid in a tank, but opens under pump pressure. The pressure setpoint is adjustable from 5 to 150 psi. Once the set pressure is reached, the valve begins to open. It will allow the rated full flow at approximately 40% over the set pressure. Anti-siphon valves are available in pipe sizes from 1/4–2 in., with various body materials, including Grade 1, Type 1 polyvinylchloride, polypropylene, Corzan, Kynar and Teflon. Flow-rates range from 2 to 75 gal/min. — *Plast-O-Matic Valves, Inc., Cedar Grove, N.J.*

[www.plastomatic.com](http://www.plastomatic.com)

### Electrical position indicators for quarter-turn valves

To automate process plants, the LSC limit switch box (photo) detects the valve position of manually and pneumatically operated quarter-turn valves. This is signaled by an optical indication and transmitted to the plant control system. The LSC position indicator can be fitted to all quarter-turn valves, such as butterfly valves or ball valves, with a VDI/VDE 3845 standard interface. — *GEMÜ Gebr. Müller Apparatebau GmbH & Co. KG, Ingelfingen-Criesbach, Germany*

[www.gemu-group.com](http://www.gemu-group.com)

Gerald Ondrey



# New Products

## See filter status in real time with this software solution

This company offers a solution for precise monitoring of the filter status of heavy-duty machinery. This type of proactive monitoring offers many advantages over common reactive measures. In the system (photo), various sensors monitor the load status of air and cabin air filters, oil, hydraulic oil and transmission oil filters, as well as fuel pre-filters and main filters. Furthermore, the status of the engine oil, hydraulic oil and fuel can be observed. The measured data are transferred from the respective machine to the OEM cloud, where it is anonymized and then passed on to this company's cloud. Algorithms analyze the data of the individual sensors and determine precise key figures for the predictive maintenance. This information is prepared and returned digitally to the OEM, which makes the information available to fleet operators and end users in the telematics system or via an application (app). — *Mann+Hummel International GmbH & Co. KG, Ludwigsburg, Germany*  
**[www.mann-hummel.com](http://www.mann-hummel.com)**

## AI improves asset monitoring and maintenance planning

The Maximo Asset Monitor (photo) is a new remote-monitoring platform powered by artificial intelligence (AI) to help maintenance and operations leaders better understand and improve the performance of their high-value physical assets. This new platform can unlock essential insights with AI-powered anomaly detection and provide enterprise-wide visibility into critical equipment performance, resulting in faster problem identification that can inform better decisions and reduce downtime. The Maximo Asset Monitor also enables users to integrate asset information and history and unify asset-management processes. With multiple deployment models, users can maintain all asset types no matter where they reside, set up new assets quickly and upgrade enterprise asset-management (EAM) software automatically without interrupting uptime. — *IBM, Armonk, N.Y.*  
**[www.ibm.com/products/maximo](http://www.ibm.com/products/maximo)**

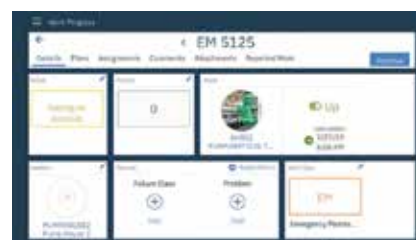
## This power supply has a new IO-Link Communication Module

The Pro 2 line of power-supply units (PSU; photo), with units ranging from 120 to 960 W, can connect to various gateways via a snap-on communication module (currently, IO-Link; Ethernet-based protocols such as Modbus TCP, Ethernet IP, ProfiNet in the future). This selection of standardized protocols ensures convenient and reliable integration into the respective infrastructure. Data from the Pro 2 PSU can be saved and analyzed for energy optimization; the central PLC can switch off distributed PSUs in parts of the system via a hardware signal or bus command in order to activate standby mode to save energy — and with the unit's monitoring functions, provide information about current power supply or connected load data, and signal errors for seamless application monitoring. This status information, which can be retrieved by the controller at any time, eliminates the need to check the output voltage manually and allows on-time maintenance of the power supply and all connected loads. — *WAGO Kontakttechnik GmbH & Co. KG, Minden, Germany*  
**[www.wago.com](http://www.wago.com)**

## Decentralized field unit for measuring water parameters

The modular Online Analysis System for measuring water quality is now also available as a compact field unit (photo). Users can set parameters and evaluate measured data via digital interfaces. The field unit can be equipped with up to six sensor cubes, which it supplies with power, and guarantees full communication with the process control system. Required parameters, such as pH, chlorine/chlorine dioxide, conductivity, redox potential (ORP) and turbidity, can be recorded at various points in the process. Using the EDIP (Efficient Device Integration Platform) and graphical programming, all the parameters of the various sensor cubes can be adapted and individual warning messages generated. Customized systems can also be set up. — *Bürkert Fluid Control Systems, Ingelfingen, Germany*  
**[www.burkert.com](http://www.burkert.com)**

Mann+Hummel International



IBM



WAGO Kontakttechnik



Bürkert Fluid Control Systems



### Software for comprehensive pipeline management

PipePatrol (photo) is a comprehensive suite of software modules for long- or short-distance single and multiproduct pipelines for oil, gas, water or chemicals, offering monitoring and protection of pipelines in all operating conditions. PipePatrol can be supplied in various configurations: eight modules cover leak detection, theft detection, stress monitoring, line-break detection, tightness monitoring, batch tracking, pump monitoring and predictive modeling. To match the application, the modules can be used standalone or individually combined, and optionally complemented by a wide range of instrumentation, cybersecurity and field-data-acquisition systems. The leak detection module uses the PipePatrol E-RTTM (extended realtime transient model) for leak detection and localization for liquids and gases. The predictive modeling module forecasts pipeline operation (for example, looking at the next 24 hours) and identifies possible threats, such as shortage in supply or pressure violations. Its offline simulation then can be used to find corrective measures, as well as for planning of optimized operation in the future. — *Krohne, Inc., Peabody, Mass.*

**www.us.krohne.com**

### New technology enables biogas optimization

The MGP261 is a new Ex-certified inline multigas measurement instrument that enables biogas plant operators to optimize the production of biogas in real time, and thereby derive greater value from biowaste. The MGP261 multigas probe is said to be the world's first in-situ biogas instrument measuring multiple gases in demanding processing conditions. The instrument combines methane, carbon dioxide and humidity measurements with the company's patented infrared Carbocap sensors in a single-gas sample cell directly inside the biogas pipeline. The MGP261 is certified for use in Ex Zone 0 and 1. This offers significant advantages over extractive gas analyzers, which require auxiliary gas-sampling pumps and gas-drying equipment. — *Vaisala Oyj, Vantaa, Finland*

**www.vaisala.com**

### High-volume twin-screw feeder delivers precision

The Model TSF twin-screw feeder (photo) is designed for precise batching and weighing applications, including: batching to weigh hoppers; low loss-in-weight, scale-monitored flow; low loss-of-weight batch applications with scales; drum and pail packout lines; and recipe-type batching by multiple computer-controlled units. The feeder's dual-helix design combines fast, high-volume filling with accurate dribble flow at the end of the cycle. Its compact design is ideal when limited space prohibits multiple individual screw units. Two helices — 1.5 and 4 in. in diameter — are mounted on a hopper. They are rated at 17 and 283 ft<sup>3</sup>/h, respectively, at maximum RPM with 100% efficient conveyable product and no slippage. — *Best Process Solutions, Inc. (BPS), Brunswick, Ohio*

**www.bpsvibes.com**

### A new volumetric feeder for additive dispensing systems

The new VMF-90D volumetric screw feeder (photo) is an automatic metering screw-feed system for mixing and dispensing dry materials into a secondary process. Among the standard features are a concentric material-conditioning overwind auger, an SCR controller that may be remotely mounted, a 4–20-mA integrated cycle timer, an alarm sensor and a vibratory agitator. Made of rugged, corrosion-resistant stainless steel, the feeder accurately dispenses most chemicals found in the water and wastewater industries at feedrates of 0.77 to 7.73 ft<sup>3</sup>/h and with accuracy to within 1% of volume. — *Scaleton Industries, Ltd., Plumsteadville, Pa.*

**www.scaletonscales.com**

### Intrinsically safe smartwatch for use in hazardous areas

The new Smart-Ex Watch 01 (photo, p. 31) is said to be the first smartwatch for use in Ex Zones 2/22 and Div. 2. Based on the Samsung Galaxy Watch, it offers a new way of hands-free communication and enables higher employee protection. The Smart-Ex Watch 01 can be combined with this company's Smart-Ex 02 and Ex-Handy 10 smart handheld devices to support the mobile worker



Vaisala



Best Process Solutions



Scaleton Industries

with a wide range of tasks in hazardous areas. The Smart-Ex Watch 01 offers the mobile worker full freedom of movement and communication. Hands-free navigation via advanced voice control or wrist gestures simplifies operation. A rotating bezel allows for intuitive scrolling through apps and instructions, even when wearing gloves. Thanks to integrated GPS and motion sensors, the Smart-Ex Watch 01 protects its wearer from the ubiquitous dangers of an industrial environment. Additionally, the sensors can be used to monitor vital signs for critical conditions. — *ecom instruments GmbH, a Pepperl+Fuchs brand, Assamstadt, Germany*  
**www.ecom-ex.com**

### **A fully integrated, loop-powered displacement transmitter**

The DT-12x Series of transmitters (photo) are loop-powered displacement transmitters that monitor displacement and vibration for a wide range of industrial machines. Devices

in the DT-12x Series are fully integrated transmitters, which means the driver (oscillator) and signal-conditioning electronics (vibration monitor) are built directly into the sensor. This greatly simplifies installation by eliminating the need and space requirements for a driver, vibration monitor and eventually a protective housing. Due to this design, the transmitter can be directly connected to a DCS or PLC using its standardized 4–20-mA output. The transmitter is loop-powered, so its 4–20-mA signal is not affected by long wiring distances, voltage drops or noise. This greatly simplifies installation even more when connecting to a DCS or PLC, since only two wires have to be connected in the current loop. — *Brüel & Kjær Vibro GmbH, Darmstadt, Germany*  
**www.bkvibro.com**

### **Rugged scales handle logistical tasks**

The AGB and AGF range of bench and floor scales (photo, p. 32) feature an in-

*ecom instruments*



*Brüel & Kjær Vibro*





Micromeritics Instrument

tegrated indicator with a durable stainless-steel housing, offering protection against dust and water. Along with an audible alarm, the color-changing display shifts during checkweighing mode for at-a-glance notification if weights are over, under or within a pre-set limit. All of these features make the AGB and AGF scales well suited for heavy-duty logistical applications in warehouses. Capacities for the AGB range from 16 to 260 lb, while the AGF's capacities range from 175 to 1,320 lb. Weighing units for the pair include grams, kilograms, Newtons, pounds, ounces and more. In addition to conventional weighing, the scales offer parts counting with preset sample sizes, percentage weighing, checkweighing and check counting. A hold function freezes the displayed weight, allowing time to elapse without losing the result. The scales also feature a zero-tracking function to ensure the display returns to a zero reading. — Adam Equipment, Milton Keynes, U.K.

[www.adamequipment.com](http://www.adamequipment.com)

### Direct, in-situ assessment of critical catalyst properties

The new in situ catalyst-characterization system (ICCS; photo) delivers high-performance test capabilities for the reliable and industrially representative investigation of catalyst behavior. By integrating with the PID Microactivity Effi catalyst-screening system, the ICCS allows researchers to efficiently quantify the impact of reactions on defining catalyst parameters, such as number of active sites. The resulting data directly support the development of more effective heterogeneous catalysts. The ICCS incorporates mass-flow controllers for fully automated gas control and a cold trap for the removal of condensable vapors. A precision thermal-conductivity detector monitors changes in the concentration of gases flowing into and out of the sample reactor. The ICCS can be connected to any microreactor testing system, even custom-made units, to deliver important information on the catalyst under test, in situ. When connected directly to the Microactivity Effi system, the ICCS allows in-situ chemisorption measurements by pulsing a probe gas using a loop valve. Analyses can be carried out on catalysts, catalyst supports and other materials without any risk of exposure to the ex-

ternal environment, since there is no requirement to discharge the sample from the reactor. This eliminates the possibility of contamination from atmospheric gases and moisture, which may damage an active catalyst and compromise data. — Micromeritics Instrument Corp., Norcross, Ga.

[www.micromeritics.com](http://www.micromeritics.com)

### New filtration media adds strength and cleanability

Introduced at Filtech (Cologne, Germany; October 22–24), Sinterflo FMC (photo) is a new metal-fiber mesh composite for filter elements. The FMC structure features integrated Bekaert Bekipor technology and is composed of random fiber webs and woven mesh structures that are sintered to form a homogenous, yet multiple-layered structure designed to deliver strength and practicality in cleaning. Alongside this range of metallic Sinterflo filter elements, the company is able to provide a full range of polymeric disposable and last-chance filters, as well as a wide range of complementary filter housings. — Porvair Filtration Group, Inc., Ashland, Va.

[www.provairfiltration.com](http://www.provairfiltration.com)

### Data connectors for Ethernet and Profinet

The new, two-piece M8 circular connectors for data transmission (photo) are well suited for compact devices, such as SCADA operator interfaces or camera systems. The four-position socket contacts feature D-coding and enable data transmission at up to 100 Mbps (CAT5 in accordance with IEEE 802.3) in Ethernet and Profinet environments. For mounting in the device wall, thread or press-in housings are available for a mechanically stable port-screw connection. When connected, the device connectors fulfill the IP67 degree of protection. Specially shielded versions are available for stringent electromagnetic compatibility (EMC) requirements. The M8 device connectors are standardized in accordance with IEC standard 61076-2-114 and are suitable for currents up to 4 A, as well as voltages up to 60 V. — Phoenix Contact GmbH & Co. KG, Bromberg, Germany

[www.phoenixcontact.com](http://www.phoenixcontact.com)

Mary Page Bailey and Gerald Ondrey



Porvair Filtration Group



Phoenix Contact



## Agglomeration Processes

Department Editor: Scott Jenkins

Greg Mehos

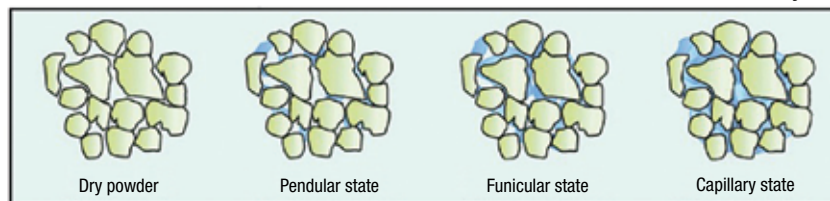
**A**ggglomeration converts fine powder particles into larger ones by introducing external forces. Major benefits for solids processors include dust reduction, easier handling, more complete utilization of raw materials and densification. Agglomerating particles happens by a variety of means, including mixing with a liquid, applying pressure and heating. This reference reviews equipment for these approaches.

### Tumble-growth agglomeration

In the first stage of wet agglomeration, fine powder, liquid and binder are combined in a mixing chamber. Fine particles are wetted with an appropriate liquid, typically water. Surfactants or other chemicals can be added to improve the wettability of the solid particles and improve pellet formation. Next, moist particles are joined together to form green (wet) agglomerates. Green particles are generated by first forming nuclei, which then grow into larger aggregates by layering or coalescence. Nucleation and aggregate growth may take place in separate pieces of equipment. For example, agglomerates from a pin mixer can be fed into a disk pelletizer. The final stage is drying or curing, which takes place in a separate device.

Binders are frequently introduced to improve the agglomerates' crush strength. In a wet tumble-growth process, powder, liquid and additives are fed continuously into the chamber, where the wetted mass is then sheared or kneaded until the liquid is evenly distributed and the granules have the desired size and strength. Examples of organic binders are waxes, rosin, starch and alginates. Inorganic binders include alkali silicates, bentonite and various aqueous solutions and dispersions. The major criteria for selecting a binder are cost, availability, compatibility with the product's final use, and its ability to give the agglomerates their desired crush strength.

Tumble-growth agglomeration equipment tends to have lower capi-



**FIGURE 1.** When liquid is added to powder, the agglomerates formed typically have their optimal strength at 40–90% of their full saturation amount

tal costs than the other methods, but costs may be higher if drying is required. Agglomerates produced by tumble-growth technologies tend to have a lower bulk density and a wider particle-size distribution as compared to other agglomeration methods. Popular wet agglomeration equipment includes pin mixers, plough mixers, disc pelletizers, fluidized beds and other technologies. Dry agglomeration is similar to wet, but it uses less wetting agent.

### Pressure agglomeration

Because attractive forces between particles intensify as the distance between them decreases, applying pressure can lead to exceptionally strong agglomerates. Pressure agglomeration falls into two general categories: roll compaction and die compaction. Roll compactors use a mechanical force to press powder. Fine particles are fed between two counter-rotating rolls, which draw material into the gap between them. The powder is compressed into a sheet if smooth rolls are used, or formed into strips if the compactor is equipped with corrugated rollers. The sheet or strips are then fed through a flake breaker. The agglomerates are irregular in shape, but often have sufficient flowability. The powder is fed by gravity or with a feeder. The equipment works best when the powder is de-aerated before it reaches the rolls. Die compaction also relies on mechanical forces to press fine powders, but also allows agglomerates with a desired shape.

Pressure agglomeration equipment tends to have higher capital costs, but lower operating costs, than tumble-growth agglomeration. Agglomerates formed by pressure have a higher bulk density, but may be more prone to attrition.

### Heating agglomeration

Extruders can heat powders to temperatures high enough to cause melting or sintering. Two types of extruders are used — ram extruders are used batch-wise, while screw extruders are for continuous processing.

In a ram extruder, powder is fed into a barrel equipped with a die plate and then isolated by a hydraulically-driven piston. The powder is then forced toward the die. The barrel may be heated (although temperatures rise due to friction, even without external heating). The entire plug of powder does not necessarily have to reach its melting point, because only a thin layer of liquid needs to be sheared between the wall and the plug. The extruder is equipped with cutters immediately downstream of the die plate. Because high pressures are generated, the feed material must have a low moisture content. Otherwise, the liquid will flash upon leaving the die plate and potentially fracture the pellets that are formed.

Auger or screw extruders comprise four sections: feed, conveying, melting or sintering, and pumping. A feed hopper contains the powder material and allows it to enter the screw beneath its outlet. The conveying section is followed by the melt or sintering section. Friction or a heated barrel increases the temperature of the conveyed powder. Pressure is generated by pumping the material through a die plate or restricted orifice. Cutters are used to convert the extrudate into pellets. ■

**Editor's note:** Material in this column comes from: Mehos, G. and Kozicki, C., Choosing Agglomeration Equipment, *Chem. Eng.*, October 2017, pp. 51–57.

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## Ethylene oxide production from ethylene

By Intratec Solutions

**E**thylene oxide (also known as EO, oxirane and epoxyethane) is the simplest cyclic ether. Because it is highly reactive, ethylene oxide is one of the most versatile chemical intermediates. It is converted into a wide range of products (for example, monoethylene glycol (MEG), surfactants and glycol ethers).

### The process

The process examined here (Figure 1) is a typical direct oxidation process in which pure oxygen is used as the oxidizing agent. The process consists of three major sections: (1) oxidation; (2) reagents recovery; and (3) product separation.

**Oxidation.** Initially, fresh ethylene, methane make-up and oxygen are mixed with recycle gas (recovered downstream). Methane is used as ballast gas to control flammable limits in the process. The mixture is heated by heat exchange with reactor effluent and fed to a multi-tubular catalytic reactor. There, ethylene oxide is selectively produced over a silver catalyst supported on alumina. The heat from this exothermic reaction generates steam on the reactor shell side, and is used for heating purposes throughout the process. Also, part of the ethylene is combusted, generating carbon dioxide and water.

**Reagents recovery.** The gaseous stream obtained from the reactor outlet is counter-currently contacted with cold water in an absorber for the separation of light gases (mainly

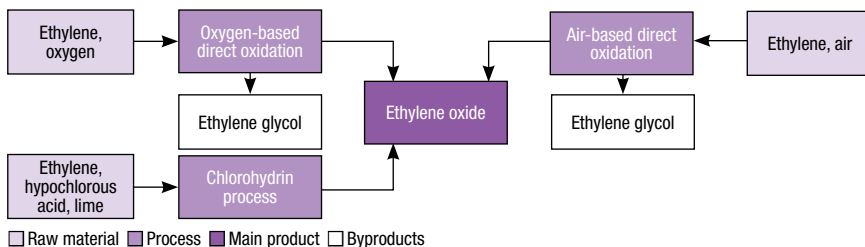


FIGURE 2. Several production pathways exist for ethylene oxide

CO<sub>2</sub>, unreacted ethylene, oxygen and methane). The bulk of the gaseous overhead stream is directly cycled back to the EO reaction by a compressor. The remainder of the gaseous overhead stream is treated for CO<sub>2</sub> removal before being sent back to the reactor. A liquid solution of EO dissolved in water is withdrawn from the absorber as a side stream.

**Products separation.** The EO/water stream from the absorber is fed to the top of a stripper, where EO is separated from water. The stripper bottoms — a water/ethylene glycol mixture — is routed to a column for recovering antifreeze-grade monoethylene glycol (MEG), which is sold as a byproduct. The overhead gaseous stream, relatively concentrated in EO, is condensed and sent to a light-ends removal unit. Crude EO withdrawn from the bottom of this unit is fed to a final purification column for the removal of water and heavy impurities. High-purity ethylene oxide (99.9 wt.%) is obtained from the column overhead and is condensed and sent to storage.

hypo-chlorous acid and the resulting chlorohydrin is dehydrochlorinated with lime, yielding ethylene oxide and calcium chloride. Currently, EO is primarily produced via the more efficient direct oxidation of ethylene, which may be air-based or oxygen-based. Different pathways for EO production are presented in Figure 2.

### Economic performance

The total operating cost (raw materials, utilities, fixed costs and depreciation costs) estimated to produce ethylene oxide was about \$520 per ton of ethylene oxide in the fourth quarter of 2015. The analysis was based on a plant constructed in the U.S. with capacity to produce 550,000 metric tons per year of EO.

This column is based on “Ethylene Oxide Production from Ethylene – Cost Analysis,” a report published by Intratec. It can be found at: [www.intratec.us/analysis/ethylene-oxide-production-cost](http://www.intratec.us/analysis/ethylene-oxide-production-cost).

Edited by Scott Jenkins

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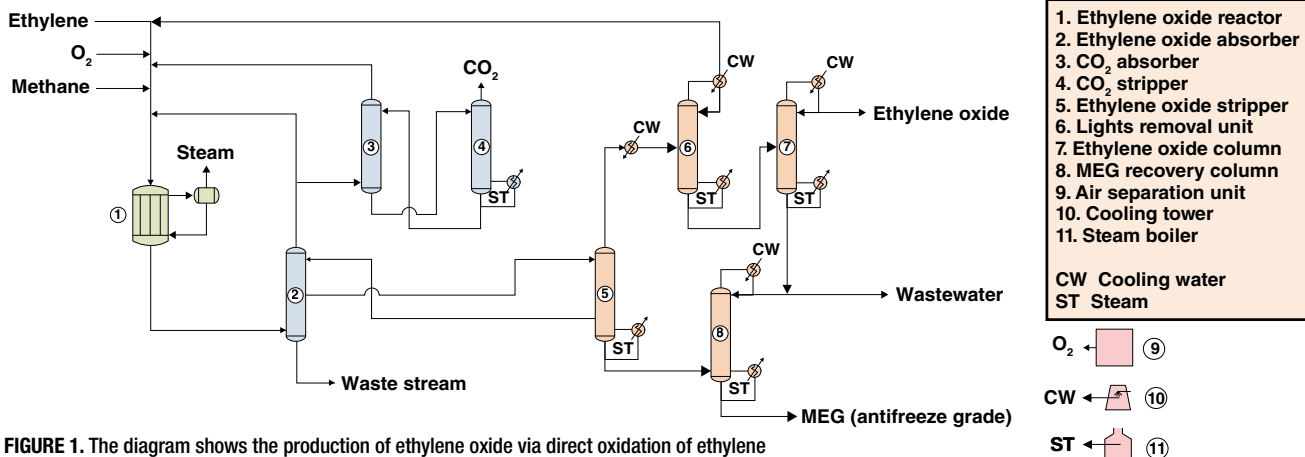


FIGURE 1. The diagram shows the production of ethylene oxide via direct oxidation of ethylene

# Storage Tanks: Snapshots of Failures, Damages and Inspections

Lessons learned from past failures provide insight and know-how needed to inspect and operate storage tanks reliably



Ana Benz  
IRISNDT

## IN BRIEF

ROOF CHALLENGES

WELDING THE DRAIN  
NOZZLE IN LARGE TANKS

CRACK IN THE FLOOR-  
TO-WALL JOINT

FIBER-REINFORCED  
PLASTIC SEPTIC TANKS

NON-INTRUSIVE NON-  
DESTRUCTIVE TESTS

ROBOTICS

Storage tanks are a common sight at many facilities of the chemical process industries (CPI). Tanks are part of our everyday life and they appear deceptively simple. However, they require a great deal of know-how and specialized knowledge to operate reliably. Otherwise, failures can occur.

Some tank failures are well known by the public, as the following examples show:

- In 1919, an accident involving a distilling tank with molasses killed 21 persons in Massachusetts [1]
- In the 1984 Bhopal tragedy, people were exposed to methyl isocyanate gas, resulting in 3,787 or more deaths [2]
- In 2001, when a sulfuric-acid storage-tank failure in Delaware City, Delaware [3] resulted in one person's death, eight others injured and significant damage to aquatic life

Although the damage and failures discussed in this article have had less impact than these well-known examples, they underline that a great deal of know-how and attention to detail are needed to operate storage tanks reliably. The tank incidents presented are the following:

- Roof challenges
- Welding the drain nozzle in large steel tanks
- Crack in the floor-to-wall joint

- Know-how for installing fiber-reinforced plastic septic tanks
- Non-intrusive non-destructive tests

## Roof challenges

**Fixed-roof tanks are designed to fail at the shell-to-roof weld.** A fixed-roof tank exploded while personnel were refurbishing equipment upstream of the tank. The roof was torn off and one of the persons working upstream was severely injured.

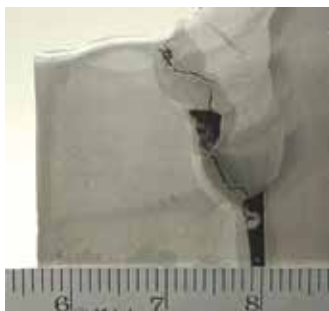
The work upstream had resulted in a pressure surge. The vents were supposed to allow the pressure to blow off, but the sudden pressurization was such that the undersized vent could not transfer gases quickly enough. The failed tank roof-to-shell weld had a torn, overloaded appearance. It appeared to be free of pre-existing flaws. The pressure at which the roof separated was estimated to be 0.6 psi. This value appeared to be low, but many tanks are constructed according to API Standard 650 "Welded Tanks for Oil Storage." Such tanks intentionally have a weak roof-to-shell seam so that if an internal overpressure from an explosion or a similar situation develops, the design allows the roof to separate from the vertical shell to prevent failure of the bottom seams and the tank's "rocketing" or propelling upward [4].

**Fixed-roof condition after removing in-**

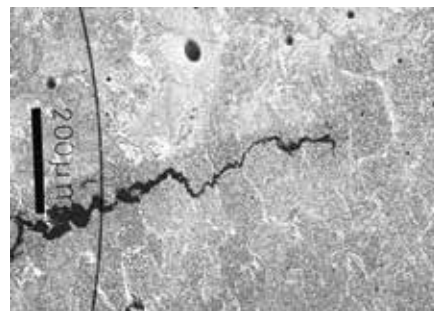




**FIGURE 1.** After removing the insulation, this tank roof showed numerous openings



**FIGURE 2.** Cracks were observed in this tank shell-to-nozzle weld



**FIGURE 3.** A closeup of the tank shell-to-nozzle fillet weld crack shown in Figure 2

**sulation.** After removing the insulation from a roof, inspection personnel identified numerous through-thickness openings in the roof (Figure 1).

**Lesson learned about fixed-roof tanks.** Do not walk on the roof without significant hazard diminishing strategies.

### **Welding the drain nozzle in large tanks**

During hydrostatic testing, an NPS 3 (nominal pipe size) tank drain nozzle leaked. The tank was fabricated to hold diesel fuel. The drain nozzle had one fillet weld joining it to the shell and another joining it to a reinforcing pad (repad), which is a plate formed

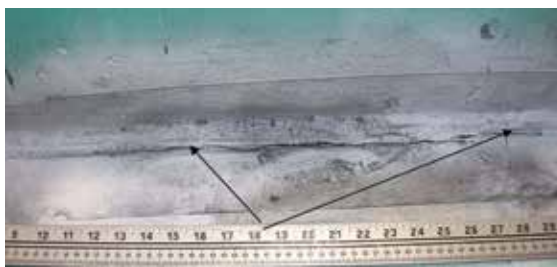
to the shape of the tank or vessel around a nozzle for extra strength. The welds had multiple cracks, porosity and non-fusion, as can be seen in Figures 2 and 3.

**Lesson learned about welding the drain nozzle in steel tanks.** Tanks are welded from the floor up. This means that access to this location (the drain) for welding is challenging. To prevent leaks, the welding passes can be deposited in multiple stages to prevent the formation of continuous leak paths. The hold times for the hydrostatic test should meet and exceed the standard requirements. Fluorescent liquid penetrant could make identifying a minute leak easier.





**FIGURE 4.** Shown here is the tank shell-to-bottom joint. Note the occurrence of soil settlement and tank wall distortion



**FIGURE 5.** Cracks of the tank wall of Figure 4 are identified with magnetic particles



**FIGURE 6.** For the same tank shown in Figure 4, this metallographic cross-section of the tank floor shows intergranular cracks with oxides/corrosion products

## Crack in the floor-to-wall joint

A fertilizer service carbon-steel tank floor developed cracks in the tank wall to tank bottom joint, as shown in Figures 4 and 5. The cracks had the following characteristics:

- The cracks developed in the cross-section with the highest stresses in the storage tank. Hydrostatic and welding residual stresses are maximum on this joint
- The cracks had some oxides/corrosion products (see Figures 6 and 7)
- The cracks were intergranular

These characteristics are consistent with the cracks being due to nitrate stress corrosion cracking (SCC). Additional stresses from the soil settlement under the tank resulted in distortion of the tank wall and floor. These stresses further contributed to the cracks forming.

**Lesson learned about the tank floor-to-wall joint.** Soil settlement needs to be monitored, and this critical joint (for carbon steels) needs inspection techniques, such as magnetic particles or eddy current, or both.

## Fiber-reinforced plastic septic tanks

New, deep-underground fiber-reinforced plastic (FRP) spiral-wound tanks had water ingress while the ground was being excavated. Prior to the inward leaks, the grade for the deep underground tanks had experienced a sudden increase in water level due to rain. The rain resulted in the tanks lifting partially (due to buoyancy) from their exca-

vated installation grade.

Examining the tanks from the inside, the shape was oval (Figure 8). Also, many of the joints were “whitened.” “Whitening” can develop when FRP is subjected to localized stresses (Figure 9). These damages suggested the tanks had experienced excessive compressive displacement during their partial lift.

The summer excavation held several surprises, as follows:

- The soil surrounding the tanks had 0.3 m × 3 m × 0.1 m chunks of ice (Figure 10). Some of these ice chunks had been pressing against the tank shell. FRP is prone to cracking when subjected to localized compressive loads
- The day before the author left the site, an intermittent underground stream was noted a couple of meters below the ground level. The flow was directed at the tanks and would have eroded the ground and support for the tanks, once installed

The damaged tanks were replaced. Soil, in accordance to strict (and necessary) installation guidelines, was used to install the replacement tanks. The flow of the underground stream was diverted away from the tanks. The replacement tanks were installed without further surprises.

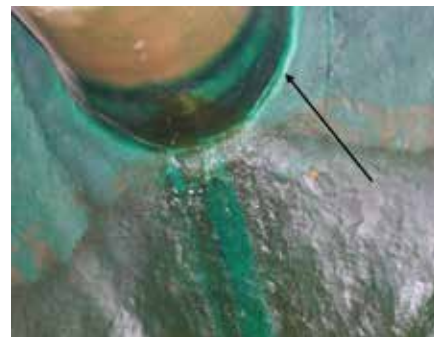
**Lesson learned about installing FRP septic tanks.** Buried FRP tanks require special installation practices heralded by their suppliers. Thorough evaluations of the soil con-



**FIGURE 7.** Another view of the metallographic cross-section of the tank floor (Figure 6), which shows intergranular cracks (2% Nital etch)



**FIGURE 8.** This septic tank's inside diameter was oval. The internals had separated from the shell



**FIGURE 9.** For the same septic tank of Figure 8, many of the inside joints had whitened — an indication of localized stress



**FIGURE 10.** During a summer excavation, large chunks of ice were identified surrounding the septic tank of Figure 8



**FIGURE 11.** Tank floor pits are identified with acoustic emission non-destructive testing



**FIGURE 12.** Using robotics for visual and coating inspections can reduce the need for personnel to enter confined spaces

ditions, underground water, grading and installation are musts.

### Non-intrusive non-destructive tests

**Acoustic emission (AE) testing of FRP and of ammonia tanks.** AE tests of FRP and ammonia tanks provide volumetric tests of shells of the tanks while in service. Entry is not required, avoiding the potentially damaging process of shutting and exposing the tanks to air (when ammonia tanks can develop stress cracks) and thermal stresses for ammonia service. The tests aim to detect and locate areas of concern. Figure 11 shows tank bottom pits identified with acoustic emission. Follow-up inspection with a complementary non-destructive testing (NDT) method is needed to identify and size any AE indications for ammonia steel tanks. FRP tanks require visual follow-up.

This technology was proven and implemented by Monsanto personnel. As stated by the author's colleague, Martin Peacock (now retired), "the initial round of testing led to shutting down several tanks for inspection and repair of fabrication defects detected by the AE test. However, once the tanks were repaired, no further inspections were required. One tank in the U.S. has been in continuous service with regular AE testing since 1984. This tank is tested every five years with the last carried out in June 2011 with no indication of service related damage to the shell" [5].

**Lesson learned about non-intrusive AE testing of ammonia tanks.** Used wisely, these tests can keep FRP and ammonia tanks operating reliably without causing inspection-related tank damage.

### Robotics

Today, we are performing robotic inspections to monitor the thickness of tank shells and roofs. Robotics are also used to inspect water tanks. The future

holds the promise of robotics being used for tank thickness, visual and various other internal inspections for multiple other services (Figure 12). This would reduce the need for personnel to enter confined spaces and the time and budgets needed for emptying and storing tank contents elsewhere. However, cleaning and navigational challenges are today the obstacles that need to be overcome. ■

*Edited by Gerald Ondrey*

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### Acknowledgements

The author is thankful for the great collaboration from many of her colleagues and customers who have allowed her to show their images. Special thanks to Chris Bishop, Martin Clements, Dustin Loveland, Dexin Lu, Martin Peacock and Marten Sales.

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# Standard ASME B16.5 Flanges: Bolt Tightening and Target Loads

Using the approach outlined here, piping engineers can select the most appropriate bolt-tightening technique based on pressure class and flange size, and calculate the required torque or tool pressure if hydraulic tensioning tools are used

**Walther Stikvoort**  
Consultant

## IN BRIEF

BOLT TIGHTENING  
SELECTION CHART

BACKGROUND AND  
SCOPE

SPECIFICS

ALGORITHM TO  
CALCULATE TARGET  
BOLT LOAD

DETERMINING TARGET  
TORQUE

DETERMINING TOOL  
PRESSURE

WORKED EXAMPLE

DISCUSSION

**FIGURE 1.** Bolted metallic flanges are a common sight on the vessels and piping systems at production plants



In the majority of industrial plants, flanged connections are used in metallic piping systems (Figure 1). The applied flanges comply with ASME B16.5 [1]. Achieving a proper preload in the bolts of a gasketed, bolted-flanged joint during joint assembly is considered crucial for its optimized performance. To realize this, various bolt-tightening techniques are available for the flange fitter. Applying appropriate tightening depends on bolt size and pressure class of the flange proper. In addition to other aspects with regard to bolted joints and their sealing performance, the appropriate and prudent choice must be made of the tightening tool and the bolt load that must be realized during assembly. This article is intended as a practical guideline for piping

mechanical engineers and focuses in particular on two specific aspects, namely:

- A selection chart that provides a demarcation between various tightening methods of bolts in standard flange connections
- An algorithm that enables the engineer involved in the design to determine the target bolt load from which the required torque or tension force can be derived

The approach described here offers the piping mechanical engineer the opportunity to select and differentiate among bolt tightening techniques for extensive piping systems based on pressure class and flange diameters. In addition, the option is offered to determine the required torque or the tool pressures if hydraulic tensioning tools are used.



Using this approach in practice, it has been shown that costs can be saved on flange assembly work without compromising safety and reliability.

### Bolt tightening selection chart

The selection chart shown in Table 1 shows the demarcation between three different bolt-tightening techniques for standard ASME B16.5 flanges. One can see that as the pressure class increases, the tightening method becomes more critical.

Table 2 is a further elaboration of Table 1, and includes the number of bolts (#) and the bolt size (size), with a color marking indicating the recommended tool type.

### Background and scope

The selection chart (Tables 1 and 2) was developed in the late 1980s at the request of the maintenance engineering department of a large exploration and production company located in the Netherlands. The core business of that company is exploring for and production of oil and gas, both onshore and offshore. The scope of the selection chart had to extend to piping pressure classes 150 to 2,500. Applicable flange materials are, successively: carbon steel, austenitic stainless steel and austenitic-ferritic (duplex) stainless steel. The chart is applicable for temperatures up to 200°C for all piping class materials. The concerned stud bolt materials are provided in Table 3.

### Specifics

Conventional hand-operated (manual) torque wrenches are specified for bolt sizes up to 1 in. Those wrenches usually deliver a maximum torque between 700 and 1,000 Nm. The bolt load accuracy for this method lies between 25 and 35%.

A bolt load accuracy of approximately 50% applies to the mechanical or hydraulic torque wrench, while an accuracy of 90% is achievable for the hydraulic bolt tensioning method.

Critical applications require special consideration. Proper tightening procedures must be strictly followed.

In some cases where hydraulic bolt tensioning is recommended, it may turn out that the use of hydraulic bolt tensioning equipment is not possible due to lack of space to install the equipment, for instance, in case of close assemblies of two valves.

In those cases, hydraulic torque wrenches are recommended provided that in addition

**TABLE 1. DEMARCATION BETWEEN BOLT TIGHTENING TECHNIQUES FOR FLANGES CONFORMING TO ASME B16.5**

Nominal diameter of flange, DN	Pressure class					
	150 (PN 20)	300 (PN 50)	600 (PN100)	900 (PN150)	1500 (PN250)	2500 (PN420)
15 (up to and including)	Use hand-operated torque wrenches without a torque multiplier device			Use mechanical torque wrench or hydraulic torque wrench		
100						
150						
200						
250						
300				Use hydraulic bolt tensioners		
350						
400						
450						
500						
600						

**TABLE 2. ASME B16.5 FLANGE BOLTING INFORMATION**

Flange size (NPS - DN)	Class 150 # - Size	Class 300 # - Size	Class 600 # - Size	Class 900 # - Size	Class 1500 # - Size	Class 2500 # - Size
½- 15	4 - ½	4 - ½	4 - ½	4 - ¾	4 - ¾	4 - ¾
¾- 20	4 - ½	4 - 5/8	4 - 5/8	4 - ¾	4 - ¾	4 - ¾
1 - 25	4 - ½	4 - 5/8	4 - 5/8	4 - 7/8	4 - 7/8	4 - 7/8
1½ - 40	4 - ½	4 - ¾	4 - ¾	4 - 1	4 - 1	4 - 1 1/8
2 - 50	4 - 5/8	8 - 5/8	8 - 5/8	8 - 7/8	8 - 7/8	8 - 1
3 - 80	4 - 5/8	8 - ¾	8 - ¾	8 - 7/8	8 - 1 1/8	8 - 1 1/4
4 - 100	8 - 5/8	8 - ¾	8 - 7/8	8 - 1 1/8	8 - 1 1/4	8 - 1 1/2
6 - 150	8 - ¾	12 - ¾	12 - 1	12 - 1 1/8	12 - 1 3/8	8 - 2
8 - 200	8 - ¾	12 - 7/8	12 - 1 1/8	12 - 1 3/8	12 - 1 5/8	12 - 2
10 - 250	12 - 7/8	16 - 1	16 - 1 1/4	16 - 1 3/8	12 - 1 7/8	12 - 2 1/2
12 - 300	12 - 7/8	16 - 1 1/8	20 - 1 1/4	20 - 1 3/8	16 - 2	12 - 2 3/4
14 - 350	12 - 1	20 - 1 1/8	20 - 1 3/8	20 - 1 1/2	16 - 2 1/4	-
16 - 400	16 - 1	20 - 1 1/4	20 - 1 1/2	20 - 1 5/8	16 - 2 1/2	-
18 - 450	16 - 1 1/8	24 - 1 1/4	20 - 1 5/8	20 - 1 7/8	16 - 2 3/4	-
20 - 500	20 - 1 1/8	24 - 1 1/4	24 - 1 5/8	20 - 2	16 - 3	-
24 - 600	20 - 1 1/4	24 - 1 1/2	24 - 1 7/8	20 - 2 1/2	16 - 3 1/2	-

The colors refer to the recommended tightening tools given in Table 1

Key:

Use hand-operated torque wrenches without a torque multiplier device
Use mechanical or hydraulic torque wrench
Use hydraulic bolt tensioners

to the use of hydraulic torque wrenches, the equal bolt stress distribution shall be controlled by means of proper bolt elongation measurements (for example, ultrasonic measuring devices).

Also, mechanical torque wrenches or hydraulic torque wrenches may be used instead of hydraulic bolt tensioning equip-



**TABLE 3. SPECIFIED BOLTING MATERIALS TO ASTM**

Diameter	Studbolts			Nuts		
[in.]	Non-sour service	Sour service	Low-temperature service	Non-sour service	Sour service	Low-temp. service
≤ 1 ½	A 193-GR.B7	A 193-GR.B7M	A 320-GR.L7	A 194-GR.2H	A 194-GR.2HM	A 194-GR.7
1 5/8 – 2 ½	A 320-GR.L7	A 320-GR.L7M		A 194-GR.7	A 194-GR.7M	
> 2 ½	A 320-GR.L43					

**TABLE 4. EQUATIONS FOR CALCULATING TOTAL REQUIRED BOLT LOAD**

Total required bolt load ( <i>W</i> ) including internal pressure ( <i>P</i> ) and external loads ( <i>F + M</i> )	Total required bolt load ( <i>W</i> ) for hydrostatic test pressure ( <i>P<sub>T</sub></i> ) without external loads	Total required bolt load ( <i>W</i> ) for gasket seating ( <i>GS</i> )
$W_{(P+F+M)}$	$W_{(PT)}$	$W_{(GS)}$
$2\pi GP (G/4 + 2bm)$	$\pi GP_T (G/4 + 2bm)$	$\pi bGy$
Required bolt load per bolt	Required bolt load per bolt	Required bolt load per bolt
$W_{(P+F+M)} / n_B$	$W_{(PT)} / n_B$	$W_{(GS)} / n_B$

#### Notation

*W* = total required bolt load, N

*G* = diameter at location of gasket load reaction\*, mm

*P* = internal design pressure, MPa

*P<sub>T</sub>* = hydrostatic test pressure, MPa

*b* = effective gasket or joint-contact-surface seating width\*, mm

*m* = gasket factor, unitless

*y* = gasket or joint-contact-surface unit seating load, MPa

*n<sub>B</sub>* = number of bolts, unitless

\*Note: Consult Table 2-5.2 of Ref. 2 for obtaining effective gasket width and diameter at location of gasket load reaction.

**TABLE 5. DATA FOR THREE FLANGES IN THE EXAMPLE**

Nominal diameter	NB 150	NB 300	NB 500
Class	600	600	600
Bolt size	1 in.	1 ¼ in.	1 5/8 in.
Number of bolts	12	20	24
Flange material	A105	A105	A105
Bolting material	A 193-GR.B7	A 193-GR.B7	A 320-GR.L7
Gasket type [4]	Spiral wound	Spiral wound	Spiral wound
Gasket dimensions, mm [4]	ID 174.8; OD 209.6	ID 327.2; OD 374.7	ID 520.7 / OD 577.9
Gasket bead, mm	1.5	1.5	1.5
Gasket width, <i>N</i> , mm	17.4 - 1.5 = 15.9	23.75 - 1.5 = 22.25	28.6 - 1.5 = 27.1
Basic gasket seating width, mm	<i>N</i> /2 = 7.95	<i>N</i> /2 = 11.125	<i>N</i> /2 = 13.55
Effective gasket seating width, mm	<i>b</i> = 2.52√7.95 = 7.11	<i>b</i> = 2.52√11.125 = 8.4	<i>b</i> = 2.52√13.55 = 9.28
Diameter at location of gasket load reaction, mm	<i>G</i> = 192.38	<i>G</i> = 354.9	<i>G</i> = 556.34
Gasket factor, dimensionless	<i>m</i> = 2.5	<i>m</i> = 2.5	<i>m</i> = 2.5
Gasket seating stress, MPa	<i>y</i> = 69	<i>y</i> = 69	<i>y</i> = 69
Grip length bolt, mm	-	-	<i>C</i> = 196.3
Nominal bolt diameter, mm	-	-	<i>D</i> = 41.275

ment in those cases where decreased operating pressures do not require high bolt stresses to maintain a reliable flange connection. In those cases, the responsible party shall provide for calculations to demonstrate the integrity of the flange connection. It is also emphasized that too low bolt stresses may lead to unstable flange connections.

## Algorithm to calculate target bolt load

When determining the target bolt load, *W*, the following loads or combinations of loads should be considered:

**Internal (design) pressure.** External loads must also be taken into account.

**Hydrostatic test pressure.** Flanged joints may be subjected to system hydrostatic tests at a pressure of 1.5 times the 38°C rating. However, the actual hydrostatic test pressure can be lower. External loads can be omitted with this condition.

**Imposed external loads.** If the magnitude of external loads is unknown, then this load may be approximated by doubling the internal (design) pressure. The background for this arises from the fact that the ratio between circumferential stress and longitudinal stress in the adjacent connected pipe amounts to a factor of two. This is equivalent to doubling the force from the adjoining cylindrical part.

**Gasket seating.** Before a tight joint can be obtained, it is necessary to seat the gasket or joint-contact surface properly by applying a minimum initial load.

Note that ASME BPVC Section VIII-Division 1 "Mandatory Appendix 2 Rules for Bolted Flange Connections with Ring-Type Gaskets," [2] is applied as much as possible.

Table 4 lists the expressions used for calculating the total required bolt load, depending on the loads mentioned above.

## Determining target torque

A common method for converting the target-bolt-assembly load into the target torque is the use of the following equation [3]:

$$T = (K \times D \times W) / 1,000 \quad (1)$$

Where:

*D* = nominal diameter of the bolt, mm

*W* = target bolt load: max [*W<sub>(P+F+M)</sub>*/*n<sub>B</sub>* ; *W<sub>(PT)</sub>*/*n<sub>B</sub>* ; *W<sub>(GS)</sub>*/*n<sub>B</sub>*], N

*K* = nut factor, to be set at 0.2 for non-coated bolts

*T* = target torque, Nm

## Determining tool pressure

The following relations are used to determine the tool pressure required to achieve the target bolt load:

$$\text{Tool pressure} = (\text{Target bolt load} \times LTF) / \text{Tool hydraulic pressure area (HPA)} \quad (2)$$

$W_{(GS)}$ , N  
 $(P+F+M)$  ;  $W_{(PT)}$  ;

$LTF$  = load transfer factor =  $1.01 + (D/C) \mapsto$  Minimum 1.1

$D$  = nominal bolt diameter, mm

$C$  = clamping or joint grip length, mm

Tensioning permits the simultaneous tightening of multiple bolts; the tools are connected in sequence via a high-pressure hose assembly to a single pump unit. This ensures that each tool develops the exact same load and provides a uniform clamping force across the joint. This is especially important for critical piping requiring even gasket compression to effect a seal. Hence, account must be taken of the simultaneous hydraulic tightening of a number of bolts (studs) to determine the required tool pressure. The pre-tension per bolt is the target bolt load or required residual bolt load divided by the number of bolts,  $n_B$ .

## Worked example

This example is based on the assumption that there are three different flange pairs, the bolts of which must be tightened with an appropriate method. The three flanges, together with their relevant flange, gasket and bolt data, are summarized in Table 5. Note that the color corresponds to the recommended tightening techniques listed in the selection chart (Table 1). The system pressures and temperatures for class 600 piping system (Group 1.1 Materials [7]) are given in Table 6.

With this information, and the equations provided above, a summary of the calculations for the three flanges is collected in Table 7. The target assembly loads and their respective hydraulic tool pressure is shown in bold font.

## Discussion

A comparison between the target torque values calculated in the example and the target torque values as stated in Table 1 of Ref. 3 is presented in Table 8. The large difference between the values calculated in the example and those according to Table 1 of Ref. 3 is due to the fact that a specific flange load situation (pressure, temperature, and so on) has been used in the ex-

**TABLE 6. SYSTEM PRESSURES AND TEMPERATURES FOR CLASS 600 PIPING SYSTEM (GROUP 1.1 MATERIALS [1])**

Design temperature, °C	Design pressure, bar / MPa	Hydrostatic test pressure, bar / MPa *	Rated pressure at 200°C, bar / MPa [7]	Rated pressure at 38°C, bar / MPa [7]
200	65 / 6.5	107.9 / 10.79	87.6 / 8.76	102.1 / 10.21

\*Note: as per applicable design code

**TABLE 7. CALCULATION FORM FOR WORKED EXAMPLE**

Nominal flange diameter	NB 150 (NPS 6 in.)	NB 300 (NPS 12 in.)	NB 500 (NPS 20 in.)
$W_{(P+F+M)}$			
$2\pi GP (G/4 + 2bm)$	657,193 N	1,894,776 N	4,214,464 N
$W_{(PT)}$			
$\pi GP_T (G/4 + 2bm)$	545,470 N	1,572,664 N	3,498,005 N
$W_{(GS)}$			
$\pi bGy$	296,503 N	646,226 N	1,119,147 N
$W_{bolt}$	657,193/12 = 54,766 N	1,894,776/20 = 94,739 N	4,214,464/24 = 175,603 N
$T = K D W/1,000$	$0.2 \times 25.4 \times 54,766 / 1,000$	$0.2 \times 31.75 \times 94,739 / 1,000$	
Target torque	278 Nm	602 Nm	Not applicable
$LTF = 1.01 + (D/C)$			$1.01 + (41.275/196.3) = 1.22$
$W_{bolt} \times LTF$			$175,603 \times 1.22 = 214,282 \text{ N}$
HPA of selected tool			3,674 mm <sup>2</sup> (*)
Tool pressure			58.32 MPa = 583.2 bars

\*Note: Hydratight tool reference number AJ4

**TABLE 8. COMPARISON OF CALCULATION VERSUS TABLE 1 OF REF. 3**

Flange identification	Bolt size	Target torque of example, Nm	Associated bolt stress, MPa	Target torque of Table 1 of Ref. 3, Nm	Associated bolt stress, MPa
Flange: NB 150 (NPS 6 in.)	1 in. - UNC	278	154	677.9	345
Flange: NB 300 (NPS 12 in.)	1 1/4 in. - 8UN	602	158	1423.6	345

**TABLE 9. THE PROBABLE BOLT STRESS,  $\sigma_{bolt}$ , DEVELOPED MANUALLY, AS CITED IN THREE CODES**

Source	ASME BPVC VIII Div.1; Appendix S	EN 13445-3-Annex G	Rules for pressure vessels (RfPV); D 0701
Bolt size: 1 in.- UNC	$\sigma_{bolt} = 310 \text{ MPa}$	$\sigma_{bolt} = 198 \text{ MPa}$	$\sigma_{bolt} = 268 \text{ MPa}$
Bolt size: 1 1/4 in. - 8UN	$\sigma_{bolt} = 277 \text{ MPa}$	$\sigma_{bolt} = 177 \text{ MPa}$	$\sigma_{bolt} = 240 \text{ MPa}$

ample, whereas for the values according to Ref. 3, use is made of a generic situation where a target pre-stress of 345 MPa (approximately 50% yield strength of bolt material) is taken as the starting point.

Another very important item in bolting design is the question of whether the necessary bolt stress is actually realized, and what special means of tightening, if any, must be employed. Most joints are tightened manually by ordinary wrenching, and it is advantageous to have designs that require no more than this. Some pitfalls must be avoided, however. The probable bolt stress developed manually, when using standard wrenches, is cited in a number of recognized codes and in the specialized literature. An overview is found in Table 9. There one can see that there is a considerable spread in probable bolt stresses for the bolt dimensions from the example. The calculated bolt stresses of 154 MPa (for the 1 in. bolt size used in the NB 150 flange) and 158 MPa (for the 1 1/4 in. bolt size used in the NB 300 flange), are significantly lower than those that can be achieved by means of simple conventional manual tightening tools (for instance, wrenches).

*Edited by Gerald Ondrey*

## References

1. ASME B16.5 - 2017; Pipe Flanges and Flanged Fittings NPS 1/2 Through NPS 24.
2. ASME BPVC VIII Div.1 - 2017; Appendix 2.
3. ASME PCC-1 - 2013; Appendix K.
4. ASME B 16.20 - 2012; Metallic Gaskets for Pipe Flanges Ring-Joint, Spiral-Wound, and Jacketed.

## Author



**Walther Stikvoort** (Address: Wagnerlaan 37, 9402 SH Assen, the Netherlands; Email: stikvoort@ziggo.nl) is a renowned principal mechanical & structural integrity consultant who has spent about 50 years in the design and design verification of pressure vessels and piping to recognized key design codes and also has significant experience in fitness-for-service engineering critical assessment (ECA) according to common FFS procedures. He has demonstrated his expertise in several key roles, such as expertise holder static equipment engineering (Authority Level TA-1) at NAM (a joint venture of Shell and ExxonMobil) (18 years) and as manager mechanical engineering at Kellogg Continental (15 years). Stikvoort worked for NRG as a senior consultant asset integrity (7 years) and for GLT PLUS (Jacobs) as a principal consultant mechanical integrity (6 years). He developed numerous engineering standards and practices focused on improving asset integrity and involved in the development and lecturing of training courses and seminars for the pressure equipment community. He is the author and co-author of various papers and articles published in recognized international journals, engineering textbooks and technical magazines. Stikvoort graduated from the Higher Institute of Technology (The Hague, the Netherlands) where he studied mechanical engineering.

# Interpreting Normalized Profitability Metrics

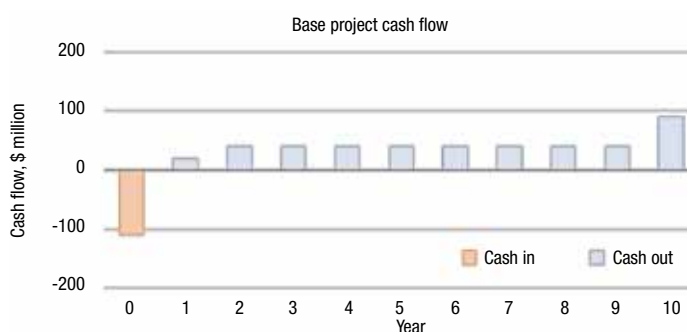
Normalized profitability metrics provide a basis for comparing the efficiency of capital investments, but they are often misunderstood. New interpretations of these metrics can help engineers to make more informed decisions

In a financial sense, a large capital project can be viewed as a series of cash flows into and out of an enterprise. The cash flows vary in timing and size, depending on the project and its characteristics. Cost engineers mathematically reduce these cash-flow patterns into discrete profitability metrics, such as net present value (NPV) and internal rate of return (IRR) so they can be more easily compared. However, such metrics are often misunderstood.

This article uses graphs to illustrate practical interpretations of three different metrics — two standard and one recently developed. Figure 1 presents a typical series of cash flows, which are the basis for the examples given in all other graphs in the article. As shown in Figure 1, cash flow for a typical capital project has four stages:

1. One to two years of negative cash flow while capital is committed
2. One or more years of subnormal cash flow during startup
3. Some period of normal operation
4. A final year with higher-than-normal cash flow, when working capital and salvage value are recovered

Two profitability metrics are needed to represent a capital project: an absolute metric and a normalized metric. The absolute metric represents the lifetime value that the project will add to the enterprise. The normalized metric represents the efficiency of the investment. While NPV is generally accepted as the industry standard for absolute metrics, there is still debate and confusion about the best choice of normalized metric.



**FIGURE 1.** All other graphs in this article are based on this typical series of cash flows for a ten-year period

For most practitioners, the default normalized metric is IRR [1, 2]. IRR is useful in certain situations, but its popularity is more likely due to organizational legacy, as well as a familiar name that suggests intuitive value. The primary alternative to IRR is modified internal rate of return (MIRR). While MIRR has gained enough traction to earn its own function in Microsoft Excel, it still mostly appears as a footnote to discussions of traditional IRR. This is unfortunate, because MIRR actually provides the intuitive value that many people attribute to traditional IRR.

This article first clarifies the practical significance of IRR and MIRR using graphs. It

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## IN BRIEF

INTERNAL RATE OF  
RETURN

MODIFIED INTERNAL  
RATE OF RETURN

NET PRESENT VALUE  
PERCENT

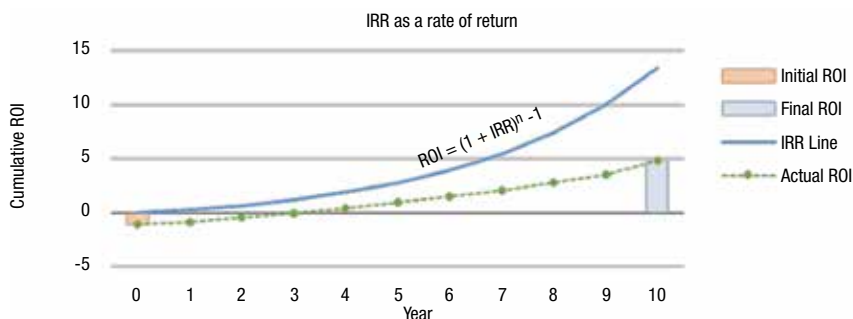
## COMPOUNDING INVESTMENTS VERSUS CAPITAL PROJECTS

This article draws a distinction between compounding investments and capital projects. Your retirement account is a compounding investment. You invest an initial principal and the principal grows over time. As principal accumulates, it grows faster. A capital project is like opening a restaurant. You invest in a kitchen, dining room, initial stock of ingredients and so on, and then each year a certain amount of people pay to eat at your restaurant.

There are two important distinctions here:

1. Unlike compounding investments, capital projects begin with an effectively non-recoverable commitment of funds
2. For a capital project, a given year's profit is effectively independent of the previous year's profit, not enhanced by it





**FIGURE 2.** When used as a rate of return, IRR can grossly overestimate the final return on the investment

then examines a third metric that follows logically from this discussion, net present value percent (NPV%). NPV% was recently proposed by D.A. Mellichamp of the University of California Santa Barbara [3] to overcome the shortcomings of IRR and MIRR. The goal of this article is to help practitioners make informed decisions regarding profitability metrics and to give them the language to explain their results to others.

### Internal rate of return

**If the project was financed at a constant compound interest rate, IRR is the interest rate at which it would break even.** IRR may be the most widely used profitability metric, but it may also be the most widely misunderstood. The name “internal rate of return” (as well as many sources) suggest that you might treat it as a rate of return on a compounding investment, like a retirement account. This comparison may be convenient, but it is not appropriate for capital projects. The box on p. 43 provides further explanation of the differences between capital projects and compounding investments. The major problem is not obvious from the

mathematical definition, as shown in Equation (1):

$$NPV = 0 = \sum_{t=0}^n CF_t(1 + IRR)^{-t} \quad (1)$$

In Equation (1),  $CF_t$  is cash flow in year  $t$  and  $n$  is project length in years. The formula can only be solved numerically, and it can have multiple, zero, or even impossible solutions, in some cases. Simply put, IRR is the discount rate for which the NPV of the project is equal to zero. “Simply put” does not always mean “simply understood” though.

It is instructive to analyze what happens when IRR is used incorrectly as a compound interest rate to calculate the final value of an investment. Figure 2 shows the actual cumulative return on investment (ROI) for the example project, alongside that calculated using IRR as a rate of return. The actual project has a lifetime ROI of 4.8, while using IRR yields a lifetime ROI of 13.4. Treating IRR as a rate of return implicitly assumes that profits can be reinvested at an interest rate equal to IRR for the remaining life of the project. This so-called “reinvestment assump-

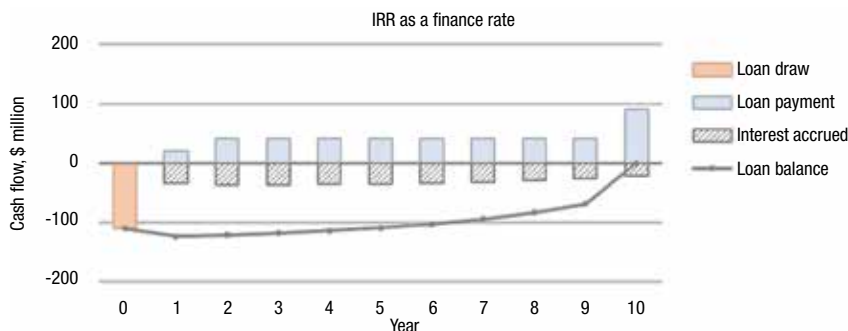
tion” has been discussed widely in literature, as well as in informal online channels. The reality is that IRR itself does not assume reinvestment. However, if you treat IRR as a rate of return, then you are assuming reinvestment.

If IRR is not a rate of return, then what is it? It can be described like this: if the project were financed at a constant compound interest rate, IRR is the interest rate at which it would break even. This statement is mathematically equivalent to the definition given above, and it is represented graphically in Figure 3. The red and blue bars represent draws from and payments to the loan — note that they are the same as the cash flows in Figure 1. The striped bars represent financing interest accrued at a rate of IRR on the previous year’s balance. The grey line represents the balance on the loan. Note that in the final year, it drops to zero. This is the break-even point.

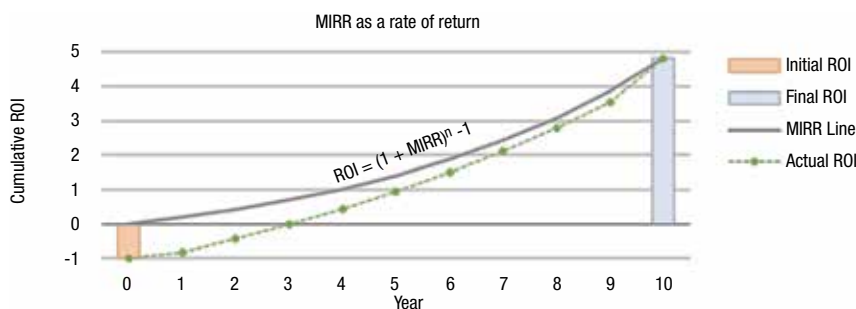
Since IRR is effectively a finance rate, it can be quantitatively compared to other finance rates, like weighted average cost of capital (WACC). WACC is the blended cost of raising funds from debt and equity. If IRR is greater than WACC, then the project will be cash-flow positive. It is difficult to extract more meaningful information beyond this, though. In an analogous sense, evaluating a project using IRR can be likened to evaluating a job offer based on the highest mortgage rate it would allow you to afford without going bankrupt in the next ten years.

### Modified internal rate of return

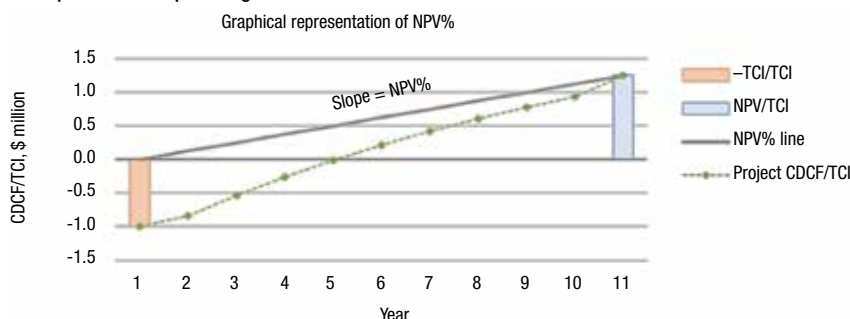
**If the project capital were put in a compounding investment, MIRR is the interest rate that would provide the same lifetime ROI as the project.** MIRR provides the intuitive value that is often attributed to IRR: it represents the interest rate on a compounding investment that would provide the same lifetime ROI as the project. Also, unlike IRR, the formula for MIRR can be solved analytically and it never has more than one solution, as shown in Equation (2):



**FIGURE 3.** If the project were to be financed, IRR is the interest rate that would produce a final loan balance of zero. Interest for each year is calculated by multiplying the previous year’s balance by the IRR. The key aspect is that the loan balance line goes to zero on the last year of the project



**FIGURE 4.** MIRR is the interest rate that would provide the same final ROI as the project, if the capital were put into a compounding investment



**FIGURE 5.** NPV% is the average percent of the investment that is added to an enterprise each year over the life of a project, as a function of the total capital investment (TCI) and the cumulative discounted cash flow (CDFC)

$$MIRR = \sqrt[n]{\frac{\sum_{t=0}^n CFI_t(1+k)^{n-t}}{\sum_{t=0}^n CFO_t(1+r)^{-t}}} - 1 = \sqrt[n]{\frac{\text{Future value of cash in}}{\text{Present value of cash out}}} - 1 \quad (2)$$

In Equation 2,  $CFI_t$  is cash flow in for year  $t$ ,  $CFO_t$  is cash flow out for year  $t$ ,  $n$  is project length in years,  $k$  is reinvestment rate and  $r$  is finance rate.

For compounding investments, MIRR is the geometric mean rate of return, but it does not retain this meaning when used for capital projects. For capital projects, MIRR's value is limited to providing a convenient way to compare compounding investments on an equal time scale. Figure 4 shows actual ROI and MIRR-estimated ROI for the example project. Both reach the same final value of 4.8, but the lines do not track one another. Actual ROI begins at  $-1$ , whereas the MIRR approximation begins at zero. Furthermore, as can be seen by comparing the slopes of the two lines in corresponding years, MIRR underestimates the yearly rate of return.

So, while the analogy is not perfect, MIRR is still a useful tool for conveying information in a world where investors often think in terms of compound interest rates. To make another analogy, evaluating capital projects using MIRR is like evaluating a job offer based on the interest rate that would earn the same amount over ten years in your retirement account.

## Net present value percent

**NPV% is the average percent of the investment that is added to an enterprise each year over the life of a project.** Capital projects do not earn compound interest — the ROI for any given year is independent of the previous year's ROI, not enhanced by it. It is therefore more

appropriate to evaluate each year's ROI in relation to the initial capital investment instead of the previous year's cumulative cash flow, and likewise, to use the arithmetic mean instead of the geometric mean. The metric NPV% is derived from these principles and can be thought of as the average percent of the investment that is added to an enterprise each year over the life of a project, as given in Equation (3):

$$NPV\% = \frac{1}{n} \cdot \frac{NPV}{PV_{TCI}} \quad (3)$$

In Equation 3,  $PV_{TCI}$  is the present value of the total capital investment and  $n$  is the length of the project in years. Figure 5 shows the graphical interpretation of NPV%. NPV% is a direct measure of the investment efficiency. Using NPV% to evaluate a capital project is like evaluating a job offer based on the average present value of your expected salary over the next ten years. Ref. 3 and 4 provide additional useful applications

of NPV%. Normalized profitability metrics provide a basis for comparing the efficiency of investments — past, present, and future. So, it makes sense to use metrics that are familiar to your organization and management team. At the same time, though, consider experimenting with other metrics like NPV% or average internal rate of return (AIRR) [5] that might prove to be more meaningful. It only takes a few extra key-strokes and can provide significant value. ■

*Edited by Mary Page Bailey*

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## How a Waste Treatment Plan Can Improve Your Bottom Line

Although waste is unavoidable in industrial processes, many companies are turning toward business strategies that seek to treat waste with minimal environmental impact — or even better, prevent waste altogether

### Aad Zwaan

Fluor

In the past, waste was simply discharged without any treatment. This occurred until authorities began enforcing regulations. Early regulations proved to be successful in reducing waste streams. However, current challenges related to declining resources and increasing energy costs require a different and more proactive approach to waste. In some cases, waste streams might prove to be a valuable product, and waste minimization, as well as energy efficiency, may be game-changing advantages for an organization. Waste minimization can be part of project execution for new-build installations, as well as revamps of existing facilities. Multidisciplinary teams can select activities to minimize waste and enhance cost efficiency. Overall, companies that invest in waste minimization as part of a sustainability strategy can financially outperform competitors who follow a less sustainable agenda.

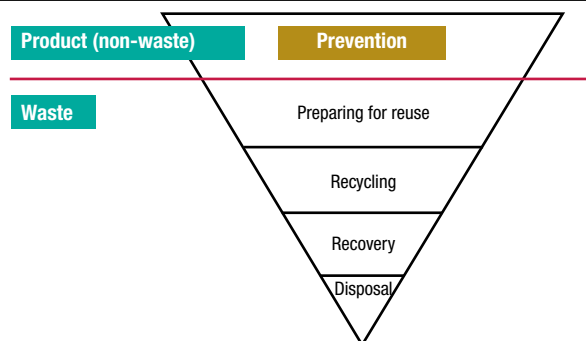
### Past practices

The industry's emphasis on waste treatment is relatively new, but industrial waste itself has a long, messy history. At the beginning of the previous century, the policy adopted by the chemicals industry for waste handling was to either dilute or isolate the waste stream [1]. The common practice was to discharge liquid waste into rivers or other water bodies for dilution and then let nature do its work. The common belief in industry was that "natural purification" would solve the problem of toxic substances in waste streams. Isolation as a policy involved selecting a remote location far away from the public to avoid nuisance and

discharge the untreated waste into rivers or to the atmosphere. These policies increasingly caused problems, as the pollution of water bodies affected the public water supply, and also as urbanization expanded near production sites.

Protection of the environment was of less importance in the past. However, under pressure from public and environmental institutions, things changed. U.S. Congress prohibited dumping oil waste into marine environments in 1924. Supervisory water boards started questioning the practice of discharging liquid waste into rivers and water bodies. Some companies were reluctant to incorporate waste treatment in those days, claiming that the costs were too high or that appropriate technology was not available. However, in the 1930s, many waste-treatment capabilities were indeed readily available. Representatives of waste-treatment providers claimed: "There is no waste discharged for which there is not a treatment," and added "what may at first seem to be an exorbitant expense in order to stop polluting, a stream may prove to be a boon to a plant by the proof to the owner that he is throwing away a product that may be of value" [1].

Nonetheless, dumping hazardous waste in pits and lagoons remained the most common practice until the 1970s. Companies would do this partially on their own property, if there was enough space, and partially on the property of others, transferring liability to other parties, as in the case of Love Canal, N.Y. [2].



**FIGURE 1.** The E.U. Waste Hierarchy provides guidance on best practices for handling industrial waste

### Progress is made

These practices were not sustainable, and under the pressure of public opinion and regulatory bodies, legislation was introduced to prevent pollution of soil, water and air. This occurred in all industrialized countries comprising the Organization for Economic Co-operation and Development (OECD; Paris, France; [www.oecd.org](http://www.oecd.org)). Waste philosophy changed, and the waste hierarchy was introduced. The waste hierarchy in the U.S. is provided by the Environmental Protection Agency's (EPA; Washington, D.C.; [www.epa.gov](http://www.epa.gov)) Sustainable Materials Management: Non-Hazardous Materials and Waste Management Hierarchy. In Europe, the European Union (E.U.) Waste Hierarchy approach was adopted in the Waste Framework Directive (2008/98/EC), which, by itself, dates back to 1975. The approach is illustrated in Figure 1.

The philosophy worked. As evidence of this, the total petroleum hydrocarbons (TPH) discharged from European refineries has declined significantly since the 1970s, as reported by Concawe [3] and depicted in Figure 2.

Over the same period, the total quantity of wastewater discharged

from E.U. refineries declined from 3.12 billion to 0.24 billion m<sup>3</sup>/yr in 2013 [4]. However, the relative, as well as absolute, quantity of hazardous waste over the same period increased to 1.07 ton/kiloton of waste versus throughput in 2013. For non-hazardous waste, the average quantity in the same year is 1.45 ton/kiloton throughput. The rise in production of hazardous waste can be explained by the proliferation of waste-emission-control facilities, such as three-stage wastewater treatment and the consequent rise in biological sludge production; or the increased use of electrostatic precipitators (ESP) to remove dust from fluegases; or an expansion in the tonnage of material removed during remediation activities [4]. Sludge and spent chemicals, including acids and bases, are the main volume of the produced waste in petroleum refineries (typically around 45% and 14%, respectively). Over the reported period between 1993 and 2013, the percentage of total disposed waste to landfill reduced from 40 to 20%. In parallel, the recycled waste increased from 18 to 34% [4]. Meanwhile, the total costs for waste disposal at E.U. refineries increased from \$80 million to \$137.2 million per year. These are simply the costs for disposal of the waste. The true cost of waste is much higher, and includes not only disposal costs, but also purchase cost of materials, handling and processing costs, management time, monitoring costs, lost revenue, any potential liabilities and post-disposal segregation activities [5].

### Finding value in waste

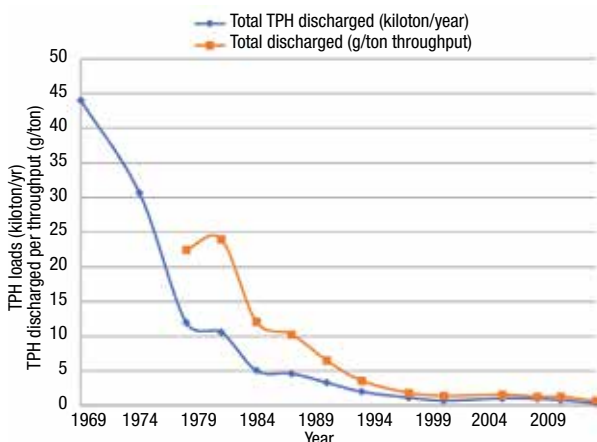
Since the 1970s, much progress has been made in waste treatment. Technology has matured and proven to be successful in reducing pollution. Waste typically has a negative connotation — nonetheless, waste can also have added value if used as a feedstock for other industrial processes. What was considered a waste stream in the past can actually be useful for certain purposes. Most refineries have included process units to treat the bottom of the barrel contents, which were previously seen as waste, producing more clean fuels and valuable products. In another example, desulfurization of natural gas and fuels generates cash flow, and has even supplanted

more traditional sulfur sources, such as the Frasch process from mining operations, as the main source of raw materials in the sulfur market (Figure 3).

Another example of waste re-purposing is petroleum coke (petcoke), which is a byproduct of extracting and processing certain types of crude petroleum. Previously seen as a waste stream that must be sent for disposal, the market for petcoke

is now expected to surpass \$25 billion by 2024 as co-incineration feed in coal-fired power plants [7]. All of these efforts were enforced by regulations, but clearly show that there are benefits to be earned in being more mindful about waste streams. As the supply of resources becomes more uncertain, minimizing waste and making more efficient use of resources as part of an overall sustainability strategy will benefit every company.





**FIGURE 2.** Coinciding with the introduction of waste hierarchy principles, total petroleum hydrocarbons (TPH) loadings and effluent rates have trended downwards significantly since the 1970s [3]

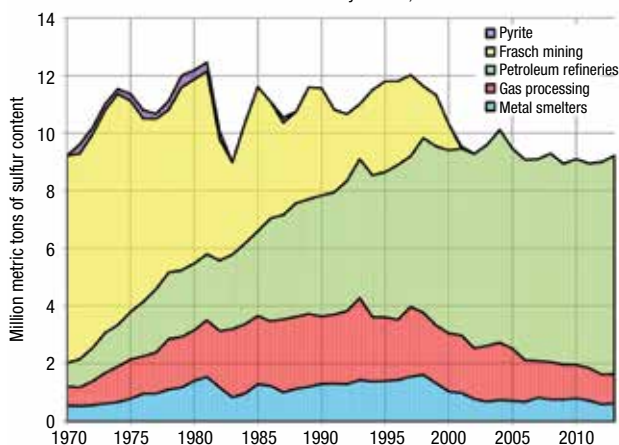
### Prevention and minimization

On top of the waste hierarchy pyramid are prevention and minimization. The best waste-treatment strategy is to not produce any waste. To enable waste minimization, there should be a shift from end-of-pipe treatment activities to adopting inherently sustainable processes throughout a facility (Figure 4). However, these efforts require careful planning and engineering. During the early phases of a project, decisions are made that affect the quantity and composition of waste. However, waste is not exclusively produced during the operational phase of the facility. Each phase of the project, such as construction, commissioning and startup, can be included in waste-management planning. A waste minimization strategy is not difficult to execute — it

simply needs appropriate attention and leadership.

There are many ways to incorporate waste minimization into a project. To succeed, sustainability efforts need to be a management priority, with clear support from a company's leadership [9]. Sustainability efforts can be implemented in both new-build and in revamp projects. Activities regarding sustainability should be assigned to a sustainability coordinator. For each project phase, a multidisciplinary team can select the most appropriate activities to devise fit-for-project solutions that serve the environment while maintaining the project's budget and operational efficiency. The engineering, procurement and construction (EPC) contractor can help support this effort by providing their expertise and knowl-

U.S. Sulfur Production by Source, 1970–2013



**FIGURE 3.** Sulfur is one example of a market where what was previously considered to be a waste-treatment operation (desulfurization units in natural gas processing) actually produces a useful raw material [6]

edge of project execution. A sample of these activities are summarized in the following sections.

**Engineering.** Selection of licenses is part of the process to minimize waste. During this process, not only capital expenditure (CAPEX) considerations should prevail, but also operating expenditure (OPEX) and costs of waste disposal and energy usage. Assuming the installation will be in operation for at least 20 years, the costs for resources, disposal of waste and energy consumption can have a significant impact on operational costs.

**Material management.** Receiving materials and equipment in the warehouses and laydown areas during the construction phase of the project produces large quantities of shipping packaging. Specifying packaging materials during the procurement of the materials and equipment can avoid significant efforts related to sorting packaging waste onsite and ensures the best possible disposal route — preferably for reuse or energy recovery.

**Construction.** Select modularization techniques to build a large portion of the project offsite in dedicated workshops — where waste can be better controlled, recycled and reused. Modularization can reduce the activities onsite and require less shipping-related packaging in comparison to having materials delivered separately for stick-built installations.

**Contracts.** Companies should require contractors to have a sustainability plan submitted as part of their technical proposal that is evaluated as part of an award recommendation. This plan would include items



**FIGURE 4.** There are opportunities to enact more sustainable operations at every level of an organization and throughout the entire lifecycle of a project [8]

such as the following:

- Water usage and recovery plan
- Energy and power usage plan
- Recycle or reuse plan for permanent and temporary construction materials
- Dust control plan
- Hazardous and toxic waste disposal plan
- Transportation plan

You may wonder: Why should I do this? The answer to this question is very simple — it's good for business. Considering waste minimization as part of a sustainability strategy provides a competitive advantage for the company [9]. A comparison made between companies operating in similar sectors (including chemicals manufacturing) with and without a strong sustainability agenda showed a considerable difference in financial performance. Companies that are more advanced in sustainability matters also have a higher return on assets (34%) and return on equity (16%) [10]. This improved performance can be attributed greatly to waste minimization and more ef-

ficient use of resources. Financial incentives are not the only benefits that come with a comprehensive sustainability strategy. Corporate image can be strengthened, as well, by showing the company's commitment to improve its sustainability. ■

*Edited by Mary Page Bailey*

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## Selecting the Right Thermodynamic Models for Process Simulation

Software that enables complex processes to be simulated continues to evolve for a wide range of thermodynamic conditions. Selection of the most appropriate models plays a crucial role in adequately representing real-life conditions

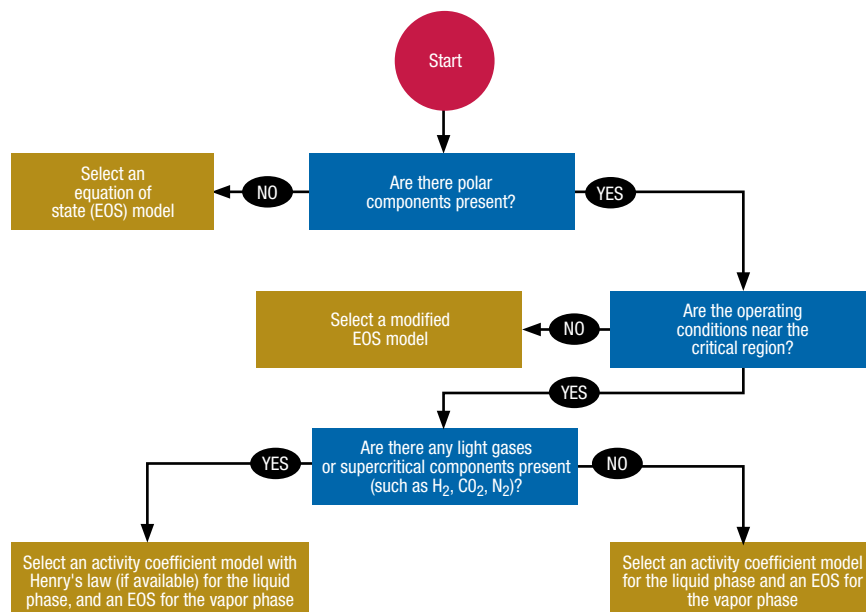
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One of the first and most important decisions to be made when modelling a chemical process system using a computer simulation package is the selection of an appropriate method for simulating thermodynamic properties. Thermodynamic-property methods enable the mathematical calculation of pressure, temperature, composition and specific volume for multi-component and multi-phase chemical systems. These calculation methods are also used as a basis for determining the state functions of a system, such as enthalpy and entropy and hence, Gibbs free energy. This article provides an overview of the primary thermodynamic-property methods, and discusses the basis that underlies each one, the strengths and weaknesses of each, and applicability of each to various chemical systems, to assist in the selection decision.

In general, thermodynamic-property methods can be categorized according to the following four options (each of which is discussed in greater detail below):

1. *Equations of state (EOS)*. These are primarily suited to describing vapor-phase behavior and predicting the vapor-liquid equilibrium (VLE) between the vapor phase and an ideal, saturated liquid phase.

2. *Liquid-activity-coefficient methods*. These have been developed specifically to model non-ideal liquid-phase behavior. These methods are more empirical in nature than EOS and therefore require more data about the system and its components. They must be used in con-



**FIGURE 1.** This decision tree can aid in the selection of the most appropriate thermodynamic method

junction with either the ideal gas equation or an EOS, to accurately incorporate vapor-phase behavior. This is sometimes referred to as a dual-model approach.

3. *Henry's Law*. Henry's Law is generally employed for environmental applications. It is applied along with liquid-activity-coefficient methods, such as non-random two-liquid (NRTL) methods. Henry's Law determines the amount of a supercritical component (non-condensable) gas in the liquid phase.

4. *Special models*. For specific applications, a specially developed thermodynamic package (for instance, having binary interaction parameters that are specially developed for the components associated with these systems) is generally available in most of the commercial simulation packages. The types of systems that are often included in these special models include

the following:

- Steam tables
- API Sour-Water Method
- Glycol
- Amines

Commercial simulation packages often use terminology such as "thermodynamic system" or "thermodynamic package" in the input data section. Selection of the most appropriate thermodynamic method is not just a decision on the thermodynamic-property method. Instead, it involves selection of all the relevant equations and methods that the simulation will use to predict vapor-liquid equilibrium (VLE), vapor-liquid-liquid equilibrium (VLLE), state functions (such as enthalpy and entropy), physical properties and transport properties.

### Equations of state (EOS)

Any equation that attempts to relate the pressure, temperature and

TABLE 1. EQUATION OF STATE (EOS) APPLICABILITY GUIDE

Classification	Low pressure	High pressure	Liquid phase	Polar molecules	Comments
Ideal gas equation	Yes	No	No	No	Strictly applicable to ideal gas systems
Generalized correlations (such as Lee-Kesler-Plocker)	Yes	Yes	No	Yes	The compressibility factor and acentric factor attempt to account for non-ideality. These correlations are of a graphical form and are easy to use. The basic premise is that all gaseous components with similar acentricity behave similarly at the same reduced temperature ( $T_r$ ) and reduced pressure ( $P_r$ )
Virial equations	Yes	No	No	No	Though these equations have reasonable accuracy for non-polar gas mixtures at low to medium pressures, they have limited applicability, as they have not been developed to the extent of the more popular cubic EOS
Cubic EOS (such as Peng Robinson (PR), SRK, RK and others)	Yes	<1,000 bar for PR, and <350 bar for SRK	Yes	No (unless specifically modified)	Cubic EOS (cubic with respect to specific volume) are the most popular EOS used in the oil-and-gas and petrochemical industries. They are relatively simple to apply and are able to predict the behavior of saturated liquid-phase components, in addition to vapor-phase behavior. They are all susceptible to errors in prediction at or very near the critical point, but are considered to be more accurate than activity coefficient methods in that region. However, by themselves they cannot predict within the two-phase (V-L) region of a pure component
More complex EOS (such as Benedict-Webb-Rubin; BWR)	Yes	Yes	Yes	Yes	Such EOS contain many adjustable parameters, which can extend their applicability, though often only for a limited range of components. Their applicability to describing liquid-phase behavior is equation-specific

specific (molar) volume of a component (or mixture of components) in a single phase can be termed an EOS. The ideal gas law represents the simplest EOS.

$$PV = nRT$$

Where:

$P$  = The pressure of the gas

$V$  = The volume of the gas

$n$  = The number of moles

$T$  = The absolute temperature

$R$  = The ideal gas constant

This equation makes no allowance for intermolecular forces, and assumes individual molecules do not occupy any volume relative to the total volume. Due to these simplifying assumptions, this EOS is only applicable to simple, spherical molecules in the gas or vapor-phase that

are present at relatively low pressure and high temperature.

In order to extend the applicability of the ideal gas equation to real gas systems and include liquid-phase pressure-vapor-temperature (PVT) behavior, a number of parameters and modifications are introduced below:

- The compressibility factor
- Acentric factor
- Van der Waal  $a$  and  $b$  correction factor
- The binary interaction parameter

Proprietary modifications to various EOS can help to extend their applicability to moderately non-ideal mixtures of components commonly encountered in oil-and-gas and petrochemical processes. For example, mixtures of glycol, alcohol, water and hydrocarbons can be described by some modified EOS. These EOS

contain binary interaction parameters, which have been determined from experimental data and actual plant operating data. Descriptions of the applicability of various EOS to various chemical systems can be found in online or in published operating manuals such as those found in Refs. 1 and 2 that accompany most commercial computer simulation packages. The general applicability of EOS methods is summarized in Table 1.

However, EOS typically have a number of limitations, which restrict their application to relatively simple and primarily non-polar components, such as hydrocarbons and light gases. The main limitations include the following:

- Complexities introduced by the mathematical methods that are used to determine the fugacity co-

TABLE 2. LIQUID ACTIVITY COEFFICIENT METHOD APPLICABILITY GUIDE

Method	Binary parameters	Different-sized molecules	Non-ideal/Polar binary mixtures	Phase splitting	Comments
Ideal solution	None	No	No	No	Only applicable to similarly sized molecules and components consisting of similar molecular species
Regular solution	None	Yes	Yes	Yes	Allows pure component data to be used to predict activity coefficients. Non-adjustable parameters attempt to account for differences in polarity and molecular size. Applicable to typical non-polar molecules such as hydrocarbons
Two-suffix Margules	One	No	No	Yes	Simplistic. Assumes all molecules are of a similar size and only considers interactions between two molecules (hence two-suffix) throughout a mixture
Two-constant Margules	Two	No	No	Yes	Assumes similarly sized molecules, but assumes that intermolecular interactions between pairs of molecules (of different molecular species) are not equal
Three-suffix Margules	Two	No	Yes	Yes	By extending the number of molecules involved in interactions to three, the range of applicability is extended. Most widely used of the Margules methods
Van Laar	Two	Yes	Yes	Yes	Does not assume similar sized molecular components, and has been extended to non-ideal mixtures. Wide usage and simple to apply
Wilson	Two	Yes	Yes	No	The main drawback is its inability to predict LLE (for instance, liquid-liquid immiscibility)
NRTL	Three -Five	Yes	Yes	Yes	Widely applicable. Good for VLE, LLE and VLLE
UNI-QUAC	Two	Yes	Yes	Yes	Parameters not as dependent on temperature as NRTL parameters. Its form makes it more applicable to solutions containing small or large molecules (such as polymers)



TABLE 3. EOS VERSUS ACTIVITY COEFFICIENT METHODS	
EOS model	Activity coefficient models
Suitable for ideal and non-polar liquids	Suitable for defining highly non-ideal liquids
Consistent property prediction in "critical" region	Inconsistent in predicting behavior near the "critical" region
Applicable for vapor and liquid phase	Represent the liquid phase only. Additionally, the gas phase must still be defined using an EOS model
Parameters can be easily extrapolated with temperature	Binary interaction parameters depend on temperature

efficient from an EOS

- Mixing rules that are used to extend the use of EOS to mixtures are somewhat arbitrary, and therefore reduce the validity of the results
- EOS are best suited to describing vapor-phase behavior. However, in combination with the advanced mixing rules, EOS can (sometimes) be used to model the liquid-phase behavior for simple and non-polar liquid mixtures. Examples for sample systems are mixtures of propane, ethane and butane and mixtures of benzene and toluene
- EOS become inaccurate at higher pressure and lower temperature, and fail to predict condensation of a gas to a liquid

### Using EOS to predict fugacity coefficients.

EOS can be used to mathematically determine the vapor-phase fugacity coefficient and, though often with less accuracy, the liquid-phase fugacity coefficient. This is done by relating the fugacity coefficient to measurable properties of pressure, temperature and specific volume through the use of residual functions. Residual functions use the thermodynamic properties of Gibbs free energy, enthalpy and entropy to mathematically describe deviations from ideal gas behavior, and can therefore be used to evaluate the fugacity coefficient of a component in a phase.

For predicting liquid-phase fugacity coefficients, semi-empirical cor-

relations, such as those by Chao-Seader (CS) and Grayson-Streed (GS), can also be used to better predict the fugacity coefficient for a range of components in the liquid phase. Thus, when used in conjunction with an EOS to predict the vapor-phase fugacity coefficient, VLE data can be predicted for systems containing light hydrocarbons and hydrogen. In fact, it is generally recommended [1] to use the GS method for systems involving heavy hydrocarbons and hydrogen, such as hydrotreating processes. It is also recommended for use in the simulation of topping units and vacuum applications handling heavy ends.

### Liquid-activity coefficient methods

Non-ideal behavior in the liquid phase is evidenced by the following:

- Strong departures from Raoult's law (which relates ideal-gas phase behavior and ideal-liquid phase behavior), due to polarity or hydrogen bond formation
- The formation of azeotropes

**TABLE 4. RECOMMENDED THERMODYNAMIC METHODS FOR VARIOUS APPLICATIONS**

Type of system	Recommended property method
Glycol dehydration	Peng Robinson (PR), specialized package
Refinery crude tower (low pressure)	Barun K10 (BK10), Grayson-Streed (GS)/Grayson-Streed Erbar(GSE), SRK/PR
Refinery crude tower (high pressure)	GS/GSE, SRK/PR
Reformers and hydrotreaters	GS/SRK/PR
Sour water	PR, sour PR, or special packages
Cryogenic gas-processing, natural gas	SRK/PR, Benedict-Webb-Rubin Sterling (BWRS)
Air separation	SRK/PR
Light hydrocarbons, petrochemicals	SRK/PR, Soave Redlich Kwong Kabadi Danner (SRKKD) for high pressure
Aromatics	Ideal for low pressure, SRK/PR for pressure greater than 2 atm
Ethylene towers	Lee Kesler Plocker (LKP), BWRS
Reservoir systems	PR/SRK
Steam systems	Steam tables
HF Alkylation	NRTL
Aromatics plus non-aromatics	NRTL/ UNIQUAC
Hydrocarbon systems where water solubility in hydrocarbon is important	SRKKD
Non-ionic, chemical applications	Wilson, NRTL, UNIQUAC
Amine system	EOS-based special packages

- The formation of two liquid phases (via liquid-liquid extraction, LLE)

The liquid-activity coefficient is essentially a correction factor that attempts to quantify deviations from ideal solution behavior. It is a strong function of composition and to a lesser extent, temperature (thus accounting for interactions between molecules), but a much weaker function of pressure. Since the activity coefficients of the components in a mixture are related to the composition, they are not independent of each other.

There are two principal approaches for determining activity coefficients for liquid mixtures:

1. Excess Gibbs free energy methods
2. Local compositional models

By estimating activity coefficients using semi-empirical or semi-theoretical equations and fitting adjustable binary interaction parameters to experimental data, VLE behavior can be predicted.

Excess Gibbs free-energy methods use excess Gibbs free energy functions, which are analogous to residual Gibbs free-energy functions in that they mathematically (and thermodynamically) relate deviations from ideal solution behavior to functions involving the activity coefficients of the components in the liquid phase. Examples of activity coefficient methods that use the excess Gibbs free-energy methodology, include the regular solution model, various forms of the Margules equa-

tion, and the Van Laar equation.

Local compositional models are semi-empirical models based on the concept that intermolecular forces will cause non-random arrangement of molecules in the liquid phase.

These models incorporate parameters related to energies of interaction and distribution tendencies of molecules, and this increases their general application and reliability while also increasing the need for binary interaction data and experimental data. Examples of activity coefficient methods that use local compositional models include NRTL methods, Wilson, universal quasi-chemical (UNIQUAC) methods and more.

A word of caution when applying liquid-activity-coefficient methods is warranted here: Due to their empirical nature and reliance on fitted parameters, liquid-activity-coefficient methods should be applied with caution, giving heed to the following criteria:

- Are components in the system common and well understood?
- Are operating conditions relatively moderate (that is, is the system at low pressure, since fitted parameter data available in commercial software packages are usually based on the assumption of ideal gas conditions in equilibrium with the liquid phase)?
- Are experimental data available and valid for the applicable range of operating conditions, either for regression to tune binary interac-

tion parameters, or to verify the predictions of the model?

If these criteria cannot be satisfied with the available experimental data, then the list of recommendations for selecting an appropriate thermodynamic property method should be consulted to ascertain whether there might be an appropriately modified EOS to describe the system. Many modified EOS are available to describe a variety of common ideal and partially non-ideal systems. In general, EOS are less cumbersome to use because of their ability to describe both vapor-phase and ideal liquid-phase behavior (unless modified to account for non-ideal behavior), and because they are less reliant on parameters that are fitted for a specific range of conditions. In any case, there is no substitute for appropriate experimental data for tuning and checking model predictions.

### Group contribution methods

When experimental data are not available, various methods can be used to predict activity coefficients based on the theory that functional groups within a molecule of any component contribute uniquely to the activity coefficient for that component. These methods are approximate because they rely on the following two simplifying assumptions:

- That the contribution of a functional group within any molecule is the same, and
- That the contribution of each functional group is independent of the contribution of any other group within a molecule

Examples of these group contribution methods include UNIFAC and ASOG. In order to apply the UNIFAC method, all components must be condensable and electrolyte solutions cannot be modeled. Given the assumptions associated with these methods, in the absence of experimental data for both the fitting of adjustable parameters and the comparison with model predictions, such methods should be used with extreme caution. From the author's experience, however, it can be stated that the data obtained from the use of UNIFAC model is not as accurate as the standard fitted values obtained from the various simulation packages.

A summary showing the general

applicability of the liquid activity coefficient methods is given in Table 2. Table 3 lists key parameters that differentiate EOS and activity coefficient models, allowing for a comparison.

### Selecting an applicable thermodynamic property method

The thermodynamic property decision tree for selecting the thermodynamic property route is shown in Figure 1.

Table 4 provides general recommendations for the selection of a thermodynamic system for modeling and simulation. These recommendations are generic in nature and are based on the author's experience and available literature [1,2]. Readers are cautioned to verify the applicability based on the operating conditions involved, and are strongly recommended to validate the simulation model. The recommended selection is intended to serve as initial guide to model the system. Further, the availability of binary interaction parameters and applicable temperature and pressure range must be verified before the selection. Readers shall note that the developers of specific simulation packages have several times modified the typical thermodynamic methods and have presented customized solutions in their software products. Readers should also take precaution to check the suitability of a particular thermodynamic method with respect to the reference and user manuals of respective simulation software.

### Concluding remarks

Commercially available simulation packages contain databases of both pure component and binary interaction parameter data. Binary interaction data can also be extended to multi-component systems. When used in conjunction with the mathematical methods pressure, temperature and phase composition can be predicted. The predictive accuracy of the thermodynamic modeling methods is dependent on both (a) the suitability of selected mathematical method(s) to describe behavior in the chemical system, and (b) the quality of the component data (pure and binary interaction) available for use in the model. ■

*Edited by Suzanne Shelley*

### References

1. PRO/II with Provision Reference Manual – Thermodynamic Property Methods Application Guidelines.
2. HYSYS User Manual: Thermodynamics: Appendix A – Property Methods and Calculations.
3. Reid, R.C., Prausnitz, J.M., and Sherwood, T.K., "Properties of Gases and Liquids," 3rd. Ed., McGraw-Hill, 1977.
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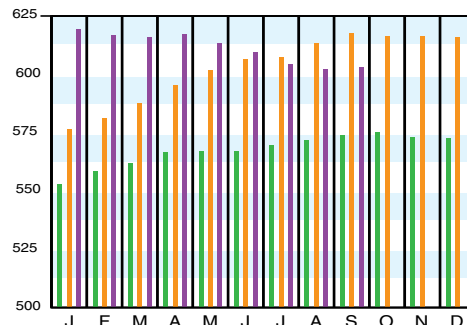
University (Aurangabad).

Download the CEPCI two weeks sooner at [www.chemengonline.com/pci](http://www.chemengonline.com/pci)

## CHEMICAL ENGINEERING PLANT COST INDEX (CEPCI)

(1957-59 = 100)	Sept. '19 Prelim.	Aug. '19 Final	Sept. '18 Final
CEIndex	602.9	602.2	617.7
Equipment	732.7	731.7	753.3
Heat exchangers & tanks	637.0	639.8	671.1
Process machinery	723.5	723.8	731.4
Pipe, valves & fittings	960.6	954.1	980.8
Process instruments	413.9	412.8	422.0
Pumps & compressors	1073.5	1071.6	1030.7
Electrical equipment	561.8	559.6	551.0
Structural supports & misc.	785.9	781.6	834.7
Construction labor	338.4	337.6	340.1
Buildings	592.3	591.8	603.7
Engineering & supervision	314.0	314.5	317.2

Annual Index:  
 2011 = 585.7  
 2012 = 584.6  
 2013 = 567.3  
 2014 = 576.1  
 2015 = 556.8  
 2016 = 541.7  
 2017 = 567.5  
 2018 = 603.1

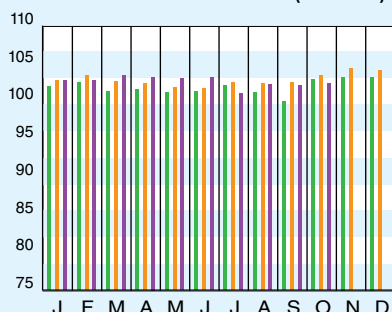


Starting in April 2007, several data series for labor and compressors were converted to accommodate series IDs discontinued by the U.S. Bureau of Labor Statistics (BLS). Starting in March 2018, the data series for chemical industry special machinery was replaced because the series was discontinued by BLS (see *Chem. Eng.*, April 2018, p. 76-77.)

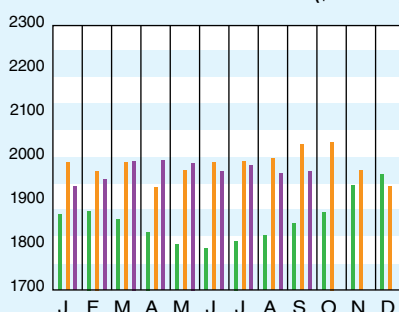
## CURRENT BUSINESS INDICATORS

	LATEST	PREVIOUS	YEAR AGO
CPI output index (2012 = 100)	Oct. '19 = 102.3	Sept. '19 = 102.6	Oct. '18 = 103.7
CPI value of output, \$ billions	Sept. '19 = 1,969.2	Aug. '19 = 1,964.3	Sept. '18 = 2,021.8
CPI operating rate, %	Oct. '19 = 76.1	Sept. '19 = 76.4	Oct. '18 = 78.1
Producer prices, industrial chemicals (1982 = 100)	Oct. '19 = 249.5	Sept. '19 = 239.8	Oct. '18 = 286.3
Industrial Production in Manufacturing (2012 = 100)*	Oct. '19 = 104.0	Sept. '19 = 104.7	Oct. '18 = 105.6
Hourly earnings index, chemical & allied products (1992 = 100)	Oct. '19 = 187.3	Sept. '19 = 184.6	Oct. '18 = 183.9
Productivity index, chemicals & allied products (1992 = 100)	Oct. '19 = 95.7	Sept. '19 = 96.4	Oct. '18 = 97.7

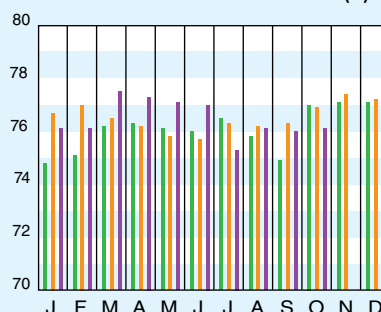
### CPI OUTPUT INDEX (2000 = 100)†



### CPI OUTPUT VALUE (\$ BILLIONS)



### CPI OPERATING RATE (%)



\*Due to discontinuance, the Index of Industrial Activity has been replaced by the Industrial Production in Manufacturing index from the U.S. Federal Reserve Board.

†For the current month's CPI output index values, the base year was changed from 2000 to 2012.  
 Current business indicators provided by Global Insight, Inc., Lexington, Mass.

## CURRENT TRENDS

The preliminary value for the CE Plant Cost Index (CEPCI; top; the most recent available) for September 2019 increased from the previous month's value by 0.7, reversing a trend of declining values this year. Three of the four major subindices — Equipment, Buildings and Construction Labor — increased, while the Engineering & Supervision subindex dipped slightly. The preliminary September CEPCI value is 2.3% lower than the corresponding value from a year ago. The magnitude of the difference in the year-on-year values increased from the previous month. Meanwhile, the CBI numbers for October 2019 (middle) show slight declines in both the CPI Output Index and CPI Operating Rate, and increased Producer Prices.